

DRAFT
GROUNDWATER MODELING REPORT
SOUTHERN CALIFORNIA CHEMICAL
SANTA FE SPRINGS, CALIFORNIA

08-28-93 4A

Prepared for
U.S. ENVIRONMENTAL PROTECTION AGENCY
WASTE COMPLIANCE BRANCH
HAZARDOUS WASTE MANAGEMENT DIVISION
Region 9
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August 24, 1993

Ron Leach
U.S. Environmental Protection Agency
Region 9
Hazardous Waste Management Division, H-4-4
75 Hawthorne Street
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Subject: Transmittal of Southern California Chemical (SCC) Draft Groundwater Modeling Report

Dear Mr. Leach:

Enclosed is the draft groundwater modeling report for SCC. The report describes the modeling approach used to assess the likelihood of detecting contamination at the facility and the results of the modeling effort. Please call Dan Ashenberg or me at (406) 442-5588 if you have any questions.

Sincerely,

A handwritten signature in cursive script, reading "David A. Donohue".

David A. Donohue
Hydrogeologist

Enclosure

cc: Neil Bingert, PRC
PRC File

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1.0 INTRODUCTION

This report summarizes PRC Environmental Management, Inc.'s (PRC) approach to computerized contaminant transport modeling at the Southern California Chemical (SCC) facility in Santa Fe Springs, California. Modeling provides information on migration of contamination from the site to assess the likelihood of detecting contamination at downgradient monitoring wells. PRC is completing this work for EPA under Technical Enforcement Support (TES) 12, Contract 68-W9-0009, work assignment 312-R09006.

PRC used a two-dimensional analytical solute transport model to predict the concentration of hexavalent chromium (Cr^{+6}) at downgradient wells along the southern boundary of the site. PRC used the public domain model SOLUTE/PLUME2D (Beljin 1989). The overall approach and application of this model differed from the model and approach used by Camp Dresser & McKee Inc. (CDM). CDM used a more sophisticated numerical model to model groundwater flow at the facility. PRC used conservative assumptions that should result in simulated groundwater contaminant concentrations higher than actual concentrations to achieve the modeling objectives.

Section 1.0 of this report provides information on site history, hydrogeology, and the objectives of this investigation. Additional details on the contamination source area and facility hydrogeology can be found in the groundwater modeling study prepared by CDM (CDM 1993). Section 2.0 discusses PRC's approach to contaminant transport modeling and model calibration at the SCC facility. Section 3.0 summarizes model results. Section 4.0 summarizes significant conclusions and discusses model limitations. Section 5.0 presents literature references used to prepare this report. A description of the model process and a mathematical statement appear in Appendix A. Model output is provided in Appendix B.

1.1 SITE HISTORY

SCC has operated a liquid hazardous waste treatment and recycling facility since 1958 in Santa Fe Springs, Los Angeles County, California. SCC receives a variety of aqueous hazardous wastes and recyclable materials from generators primarily in the electronics and aerospace industries. Wastes managed by SCC include spent etching compounds, solder strippers, pickling acids, plating

solutions, conditioners, and brighteners. These solutions contain copper, iron, lead, chromium, nickel, sulfates, and chlorides.

1.2 HYDROGEOLOGY

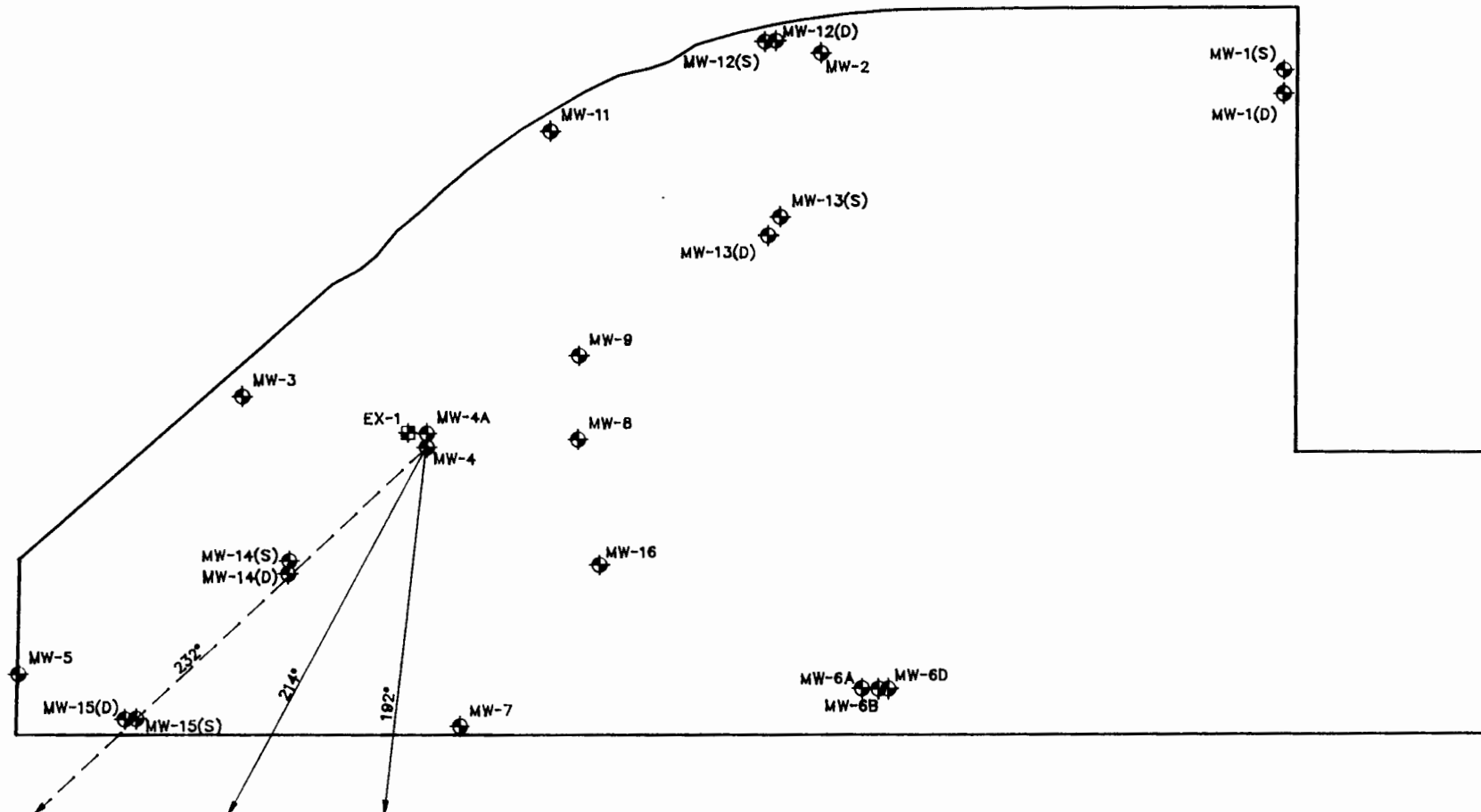
The upper and lower Hollydale aquifer is the aquifer of principal concern in this investigation. The top of the Hollydale aquifer is located approximately 55 feet below ground surface. It is composed of sands and minor silty sands with an average thickness of 40 feet. In some places, a thin clay layer up to 5 feet thick separates the Hollydale aquifer into the upper and lower aquifers. The horizontal hydraulic gradients calculated using January and April 1993 on-site groundwater elevation data is 0.0042 feet per foot (ft/ft). The apparent direction of groundwater flow is southwest, as shown in Figure 1. The calculated gradient direction for the upper Hollydale aquifer varied from Theta (Θ) equal to 192° to Θ equal to 214° . The calculated gradient direction for the lower Hollydale aquifer is 232° .

1.3 OBJECTIVES

The specific objectives of groundwater modeling at the site are to: (1) assess whether the locations of monitoring wells MW-7, MW-15(S), and MW-15(D) will detect a release off site, and (2) evaluate whether the plume will be attenuated by advection and dispersion to detection limits or below at the property boundary. Model results obtained from this investigation can only be used to evaluate the objectives stated above. Previous modeling investigations by CDM at the site used a different modeling approach to evaluate the groundwater flow system (CDM 1993). These data were then input into a contaminant transport model to predict contaminant plume conditions at the facility.

2.0 MODELING APPROACH

The sequence of activities comprising the modeling effort for the SCC facility consists of (1) developing a conceptual model of site hydrogeology; (2) selecting appropriate computer software (model code) based on the stated objectives, data availability, and budgetary constraints; (3) calibrating the contaminant transport model for Cr^{+6} ; and (4) simulating contaminant transport at the SCC facility. The results of model simulation are presented in Section 3.0.



LEGEND

- GRADIENT DIRECTION IN UPPER HOLLYDALE AQUIFER
- - - GRADIENT DIRECTION IN LOWER HOLLYDALE AQUIFER
- ⊕ EXISTING MONITORING WELL LOCATION
- ⊞ EXISTING EXTRACTION WELL LOCATION

40' 0 40' 80'
SCALE: 1" = 80'

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FIGURE 1
HYDRAULIC FLOW GRADIENT DIRECTIONS

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2.1 SITE CONCEPTUAL MODEL

Before the computer model was selected and calibrated, a conceptual model of the hydrogeology at the SCC facility was formulated. A conceptual model describes the components of a groundwater flow system and is developed from regional, local, and site-specific data. Flow system components include groundwater flow direction and gradient, aquifer thickness, and water transmitting properties. A conceptual model is a precursor to a computerized groundwater model.

The conceptual model was formulated to organize existing field data so that the groundwater flow system could be analyzed more readily. The conceptual model was simplified as much as possible. However, enough complexity was retained to simulate groundwater system behavior for the intended purpose of modeling (Anderson and Woessner 1992). The conceptual model for the SCC facility was developed using physical data and information provided in the groundwater modeling study prepared by CDM (CDM 1993a) and the quarterly monitoring report (CDM 1993b). The following assumptions were used to develop the site conceptual model:

- The aquifer is homogeneous, isotropic, and infinite in areal extent.
- Groundwater flow is horizontal and unidirectional under steady state flow conditions.
- Precipitation recharge to the aquifer, biodegradation, and recharge to the aquifer from losing streams are insignificant.
- All groundwater contamination exists in the dissolved phase.
- The average hydraulic conductivity is 267 feet per day (ft/d) (CDM 1993a).
- The saturated thickness of the aquifer mixing zone is 73 feet at MW-14 (CDM 1993a).
- The average hydraulic gradient is equal to 0.0042 ft/ft (CDM 1993a).
- The hydraulic gradient direction Θ ranges from 192° to 232° west of south (CDM 1993b).
- The aquifer porosity is estimated to equal 0.30.

- The groundwater seepage velocity is approximately 3.74 feet per draft (ft/d). This estimate is based on an average hydraulic conductivity of 267 ft/d, a hydraulic gradient of 0.0042 ft/ft, and an effective porosity of 0.30, using a variation of Darcy's law (Fetter 1980).

$$V_s = (K \times I)/n_e \quad (1)$$

where

V_s = seepage velocity (ft/d)
 K = hydraulic conductivity (ft/d)
 I = hydraulic gradient (ft/ft)
 n_e = effective porosity (unitless)

- The longitudinal dispersivity is 20 feet; the transverse dispersivity is 2 feet (Gelhar 1986).
- The retardation coefficient for Cr^{+6} is 1 (no retardation).
- Source release to the aquifer from the unsaturated zone is continuous and constant for 10 years.

2.2 MODEL SELECTION

An analytical modeling approach to the solute transport groundwater modeling was selected to keep the approach simple and cost effective. Use of an analytical approach is consistent with the amount and type of data available and the objectives of the modeling assignment. To meet the stated objectives, the well-documented, public-domain groundwater model SOLUTE/PLUME2D was used (Beljin 1989). SOLUTE/PLUME2D is distributed by the International Groundwater Modeling Center (IGWMC) in Golden, Colorado. The selection of SOLUTE/PLUME2D was based on the required level of technical detail and data availability.

SOLUTE/PLUME2D simulates the concentration distribution of a contaminant in a homogeneous, isotropic aquifer. The model handles multiple point sources that are characterized by either continuous or slug injection. In addition, the model simulates the effects of advection, dispersion, decay, and retardation. The model is based on the Wilson and Miller (1978) equations. A complete description of the governing equations, boundary conditions, initial conditions, and mathematical processes is provided in Appendix A.

SOLUTE/PLUME2D model simulates unidirectional groundwater flow. Variations in the direction of the hydraulic gradient direction across the western section of the SCC facility were accounted for by modeling various hydraulic gradient directions based on measured upper and lower Hollydale aquifer gradients. The results of multiple simulations for the hydraulic gradients were incorporated into a digitized base map at an identical scale using calculated hydraulic gradient directions to orient the plume center line.

2.3 MODEL CALIBRATION

Calibration is the process of adjusting the parameters of a groundwater flow or contaminant transport model so that the model simulates the observed aquifer data as best as possible for given (measured) parameters (such as well contaminant concentrations). The contaminant transport model for Cr^{+6} was calibrated by comparing model output to water quality field data collected in October 1990 from wells MW-4, MW-7, MW-14, and MW-15. The October 1990 data were used in the model because they provided a conservative estimate. The field water quality data from more recent sampling indicates a decrease in concentration with time since October 1990.

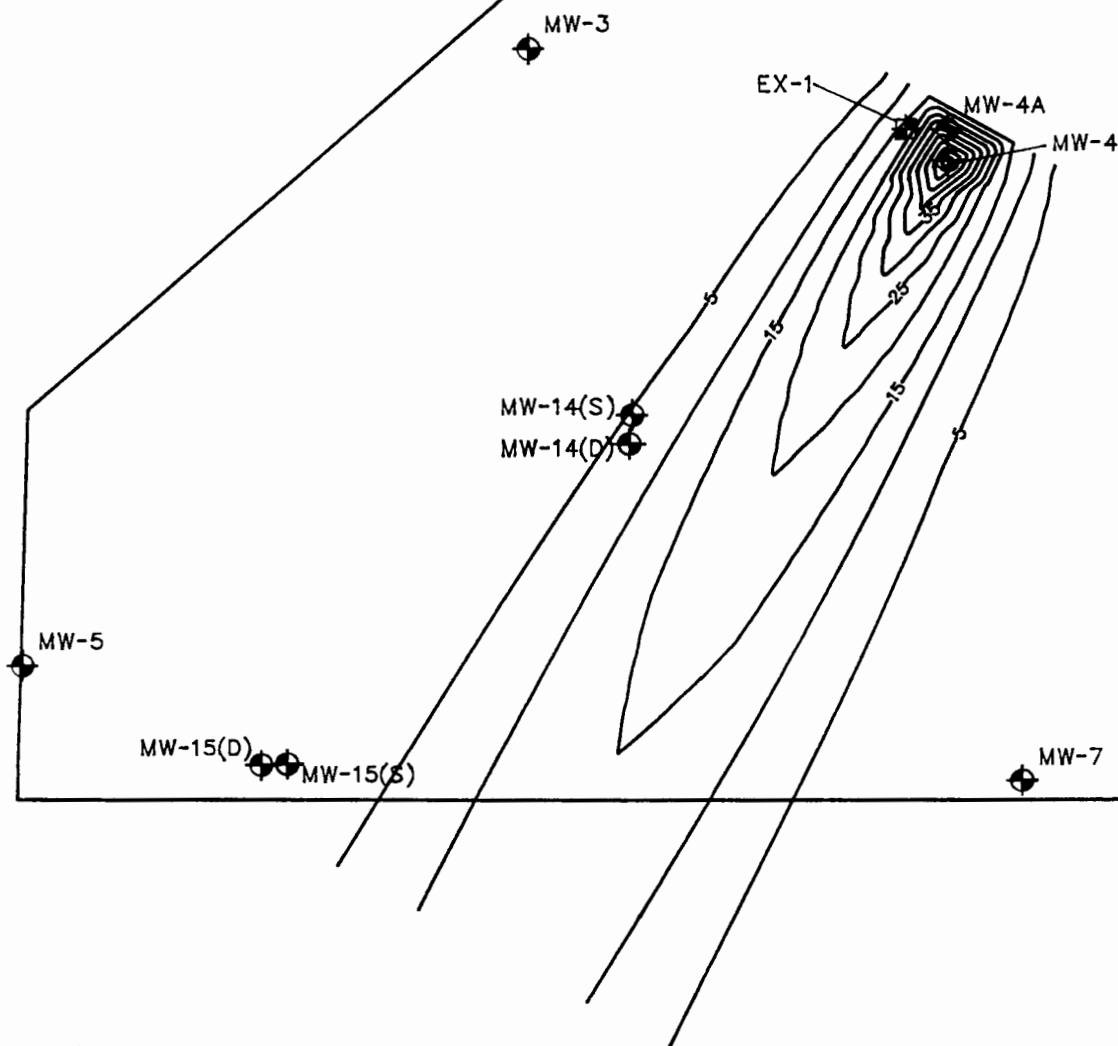
The calibration process consisted of varying hydraulic parameters until a best match was obtained when compared with known field conditions. The process was terminated when a regression analysis of field data and simulated model results for available calibration targets yielded a correlation coefficient (r^2) that was greater than or equal to 0.85 (Anderson and Woessner 1992). Hydraulic gradient directions of 192° , 214° , and 232° were used in the calibration process. The r^2 value obtained from the calibration simulations for a hydraulic gradient direction of 214° ranged from 0.995 to 0.999. Calibration using the October 1990 data as a target is reasonable based on the stated objectives for this assignment.

3.0 RESULTS

The extent of Cr^{+6} contamination was estimated using the calibrated model. Three simulations were performed by varying the hydraulic conductivities and the longitudinal and transverse dispersivities. A sensitivity analysis was performed on hydraulic conductivity (K), longitudinal dispersivity (D_L), and transverse dispersivity (D_T). The input data for the three simulations are shown in Table 1. Figure 2

TABLE 1
CONTAMINANT TRANSPORT MODEL INPUT PARAMETERS

Aquifer-Specific Parameters	Model Value			Units
	Run 1 Average	Run 2 Conservative Case	Run 3 Worst Case	
Hydraulic conductivity	267	55	307	Feet/day
Mixing depth	73	73	73	Feet
Transmissivity	19,491	4,015	22,411	Square feet/day
Porosity	0.3	0.3	0.3	---
Hydraulic gradient	0.0042	0.0042	0.0042	Feet/foot
Seepage velocity	3.74	0.77	4.30	Feet/day
Gradient direction	variable	variable	variable	Degrees
Longitudinal dispersivity	20	10	30	Feet
Transverse dispersivity	2	1	3	Feet
Source-Specific Parameters	Model Value			Units
Number of sources	1	1	1	---
Source type	point source	point source	point source	---
Loading type	continuous	continuous	continuous	---
Loading period	3650	3650	3650	Days
Loading rate: Cr ⁺⁶	4.73	0.7	6.72	Pounds/day
Decay rate	No decay	No decay	No decay	
Chemical-Specific Parameters	Model Value			Units
Retardation coefficient	1	1	1	---



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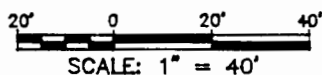
EXISTING MONITORING WELL LOCATION



EXISTING EXTRACTION WELL LOCATION



CHROMIUM PLUME CONCENTRATION
CONTOUR (mg/L)



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FIGURE 2
SIMULATED MODEL RESULTS, RUN 1
HYDRAULIC GRADIENT DIRECTION=214°

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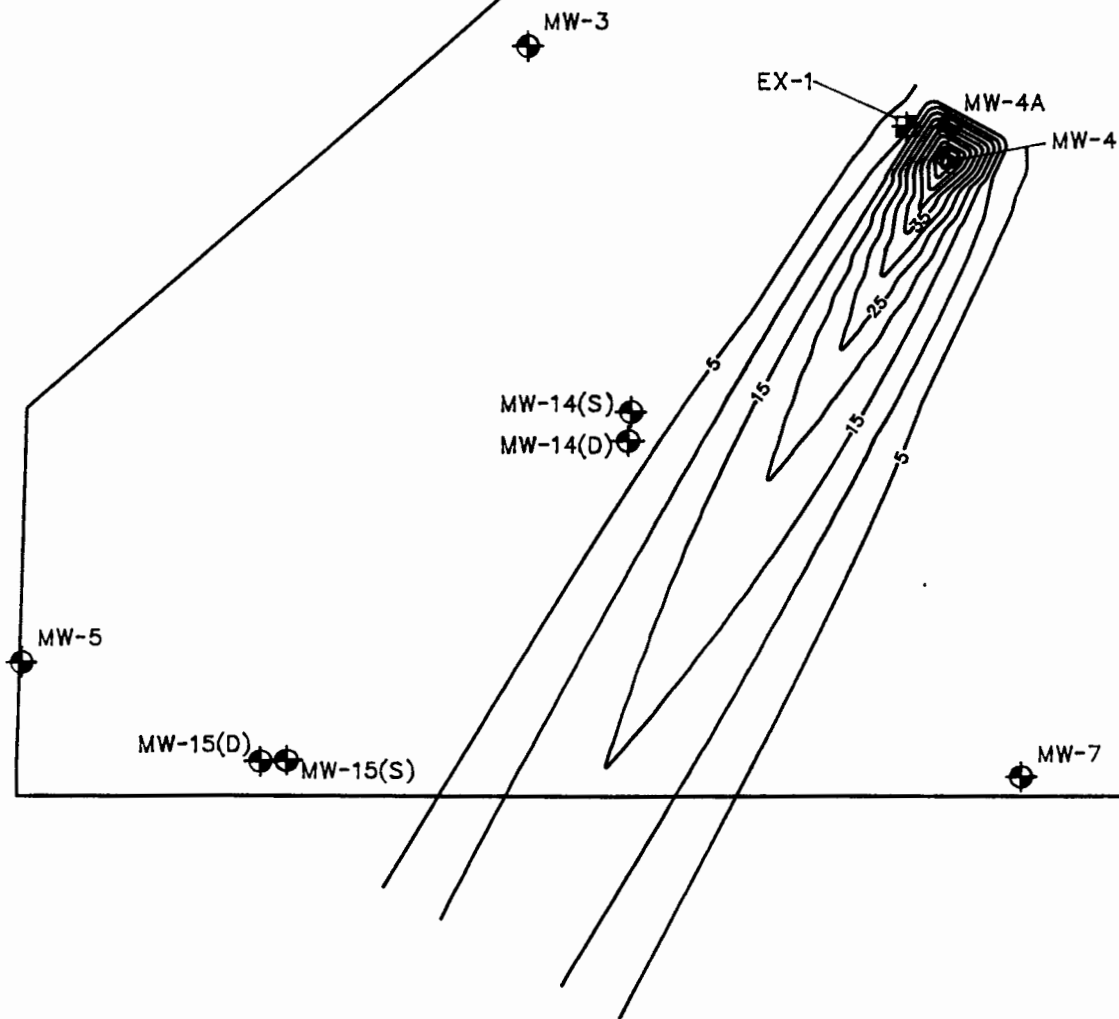
presents the results of Run 1 using average case conditions. Figures 3 and 4 present the results of Run 2 for a conservative case condition and Run 3 for an estimated worst case condition, respectively. In all three runs, the plume is oriented along hydraulic gradient direction $\Theta = 214^\circ$.

Based on modeling output, the following results were obtained:

- Dispersion modeling using simplified assumptions indicates that a plume resulting from a constant and continuous source near well MW-4 will be detected in well MW-14 under simulated groundwater flow directions.
- MW-07 and MW-15 are located on the boundary of the simulated plume when Θ is assumed to be 214° . The simulated concentrations at these locations are at or below detection limits.
- Potentiometric surface maps prepared by CDM (1993b) indicate that groundwater in the lower Hollydale aquifer exhibits a hydraulic gradient direction equal to 232° based on January and April 1993 data. Shallow Hollydale aquifer gradients appear to vary between 214° and 192° , based on January 1993 and April 1993 data, respectively (see Figure 1).
- The best model calibration was obtained when $\Theta = 214^\circ$.
- The width of the simulated plume at the southern boundary is affected by variations in assumed values for K , D_L , and D_T (Table 2). Contaminant concentrations did not vary significantly.
- The model source term was assumed to be constant and likely overestimates the concentration of Cr^{+6} in the aquifer. Field data indicate the concentration of Cr^{+6} in the aquifer has decreased with time, as shown in Figure 5.
- There are insufficient chemical data to document an off-site release. The possibility exists that a slug of Cr^{+6} may have migrated undetected between wells MW-07 and MW-15, assuming $\Theta = 214^\circ$.

4.0 CONCLUSIONS AND RECOMMENDATIONS

The fate and transport of Cr^{+6} contamination in groundwater was modeled for the western portion of the SCC facility. An analytical groundwater model was used to simplify the field situation, satisfy the stated objectives of modeling, and meet both time and budgetary constraints. The analytical model for Cr^{+6} was conceptualized, developed, and calibrated. Predictive simulations suggest that the concentrations of Cr^{+6} at downgradient wells are on the margin of the simulated plume. In addition,



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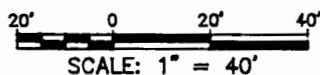
EXISTING MONITORING WELL LOCATION



EXISTING EXTRACTION WELL LOCATION



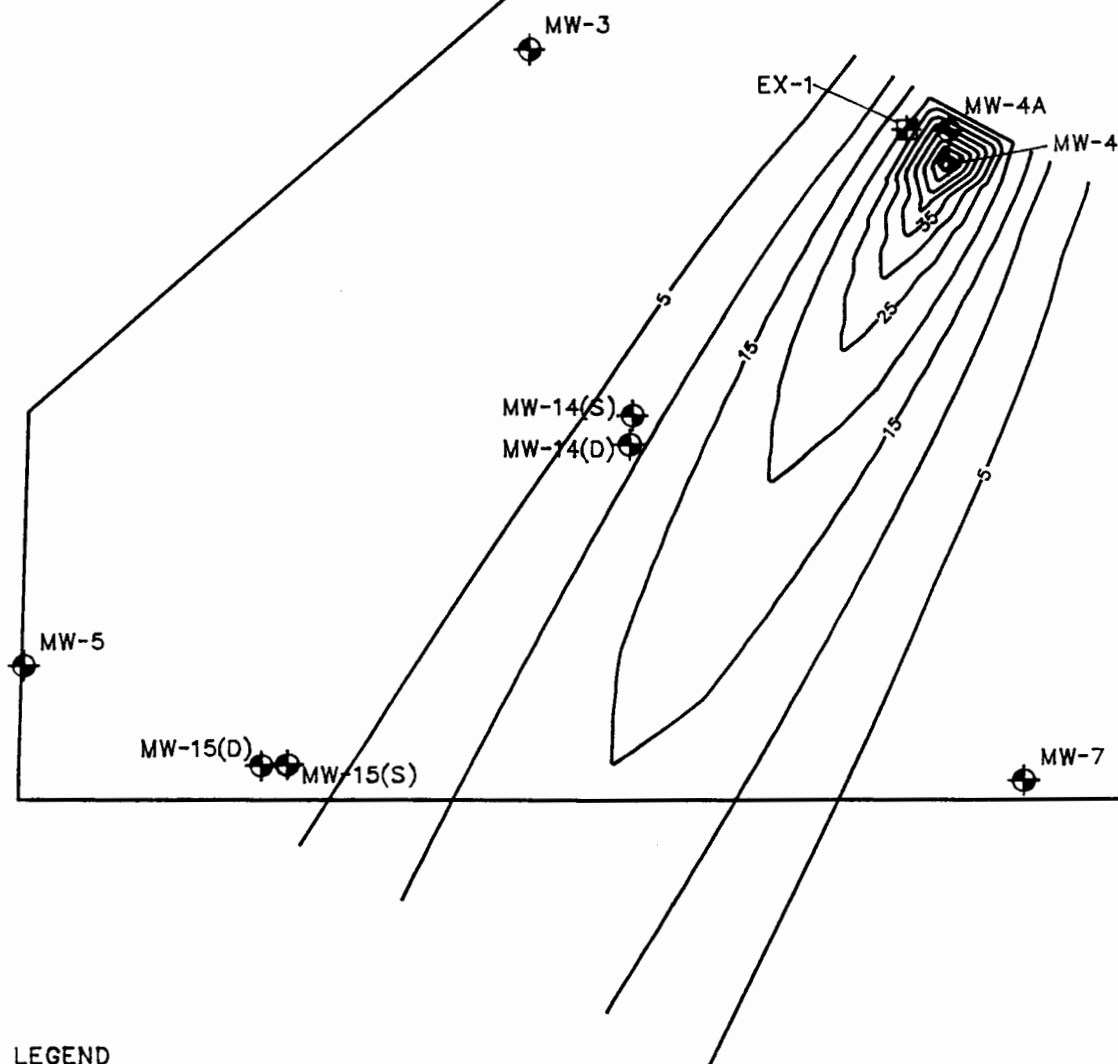
CHROMIUM PLUME CONCENTRATION
CONTOUR (mg/L)



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FIGURE 3
SIMULATED MODEL RESULTS, RUN 2
HYDRAULIC GRADIENT DIRECTION=214°

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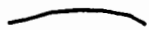
LEGEND



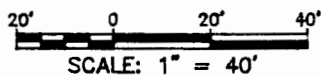
EXISTING MONITORING WELL LOCATION



EXISTING EXTRACTION WELL LOCATION



CHROMIUM PLUME CONCENTRATION
CONTOUR (mg/L)



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FIGURE 4
SIMULATED MODEL RESULTS, RUN 3
HYDRAULIC GRADIENT DIRECTION=214°

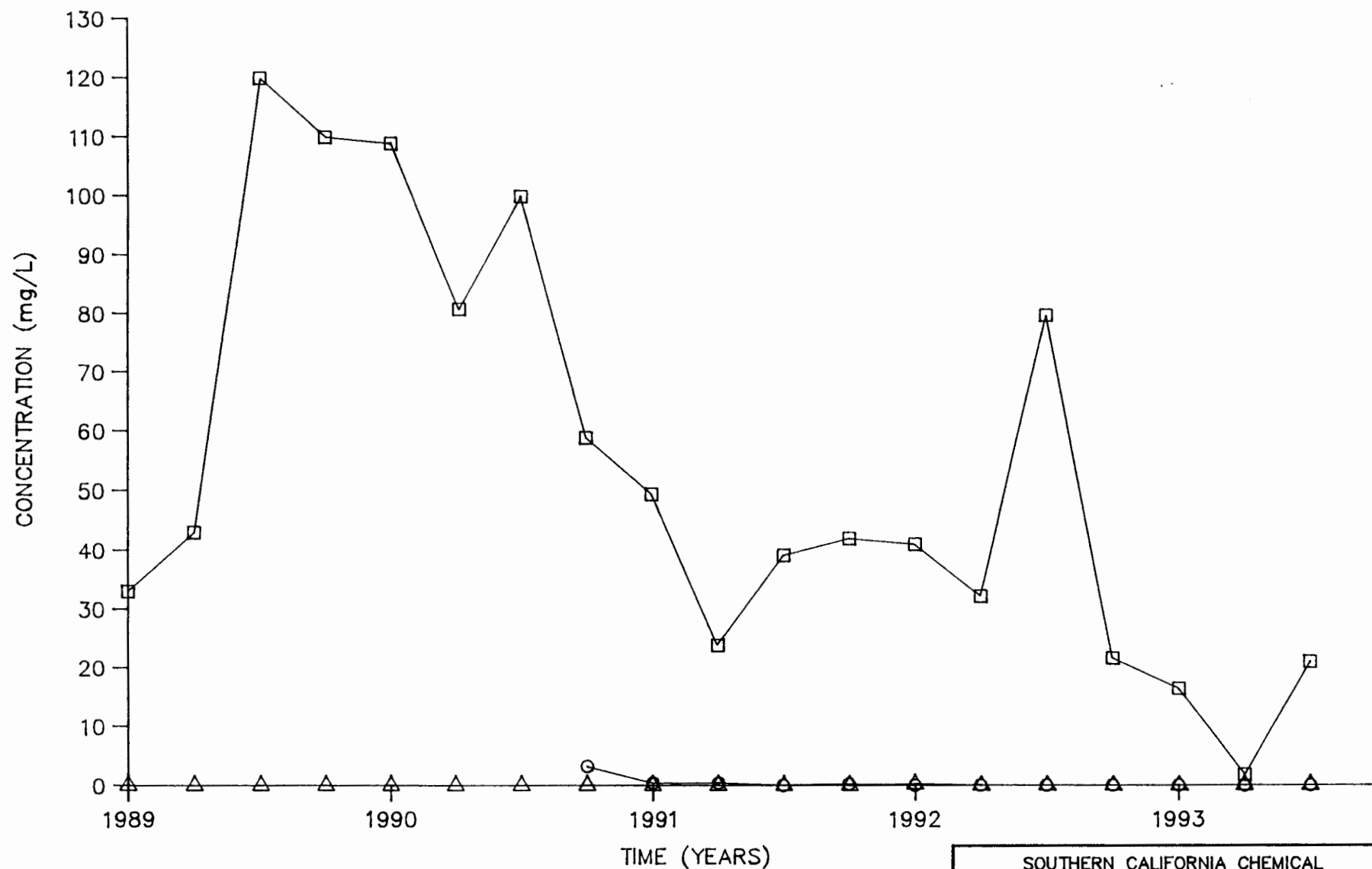
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TABLE 2

EFFECTS OF VARIOUS INPUT PARAMETERS ON PLUME WIDTH

		Run 1 Average Case	Run 2 Conservative Case	Run 3 Worst Case
Input Parameter	K	267 ft/d	55 ft/d	307 ft/d
	D _L	20	10	30
	D _T	2	1	3
	Seepage Velocity	3.74 ft/d	0.77 ft/d	4.30 ft/day
Model Simulation Results	Plume width	200 ft	140 ft	300 ft
	Maximum Concentration at Southern Boundary	15.3 mg/L	15.3 mg/L	15.2 mg/L

mg/L = milligram per liter

**LEGEND**

- MW-4
- △ MW-7
- MW-14(S)

NOTES:

ALL MW-15(S) CONCENTRATIONS WERE BELOW DETECTION LIMITS.

MW-7 CONCENTRATIONS WERE BELOW DETECTION LIMITS EXCEPT FOR JANUARY 1992.

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FIGURE 5
CONCENTRATION VS TIME IN MONITORING
WELLS MW-4, 7, AND 14(S)
JANUARY 1989 THROUGH JULY 1993

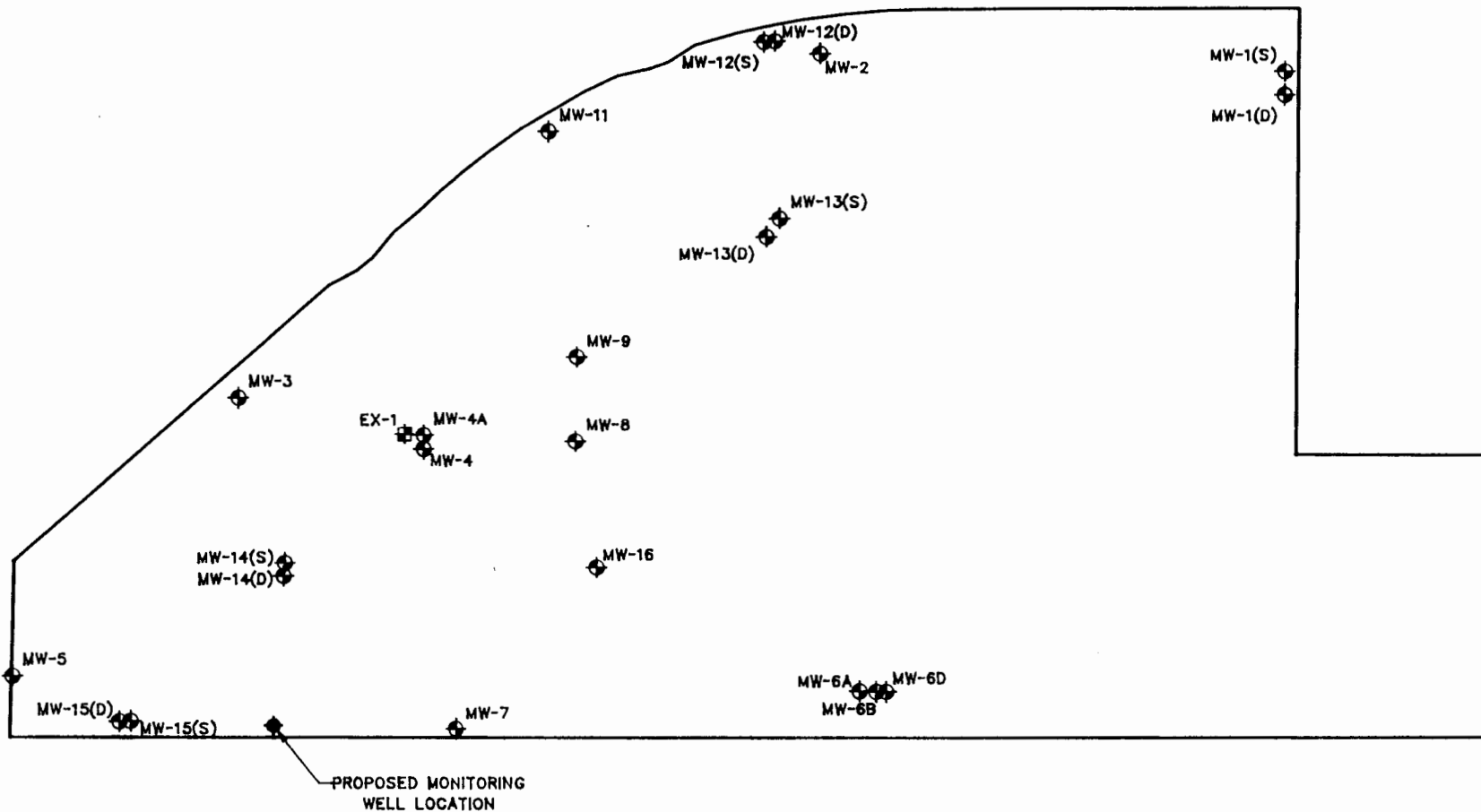
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the field data show that the concentration of Cr^{+6} in the aquifer has decreased with time. If this trend continues, there is less need to consider on-site pump-and-treat remediation. As shown from model simulation results, MW-14 is located in a critical position to detect a contaminant release from the potential source area. However, if the concentration of Cr^{+6} increases during two consecutive water quality monitoring events, a new monitoring well should be installed along the southern boundary of the facility. The proposed location is shown in Figure 6. This well would be used to obtain chemical data to document a release.

The development of the analytical transport model for the SCC facility involved numerous assumptions and simplifications. These assumptions and simplifications are listed in Section 2.1 of this report. Application of this model is restricted by the data and current knowledge of site hydrogeology. Additional field data are required to better define loading rates, estimate aquifer heterogeneities, and further characterize plume boundaries. If future investigations indicate that modifications to model assumptions are necessary, the model should be recalibrated and updated with the new data.

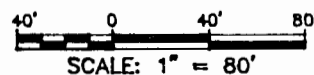
By using conservative assumptions and model parameters, the model overestimates the concentrations of indicator chemicals compared to those concentrations measured in the field. However, the current modeling results are adequate to satisfy the primary objectives of this report. These results are useful to (1) evaluate the location of monitoring wells MW-7, MW-15(s), and MW-15(D) to assess whether their locations will detect a release off-site, and (2) evaluate whether the plume will be attenuated by advection and dispersion to at or below detection limits at the property boundary. The results of modeling can be used to site future monitoring well locations, if needed. The results of modeling should not be used to identify the exact location and concentration distribution of contaminants, fill gaps in the existing data base, or simulate two- or three-dimensional groundwater flow and contaminant transport at the facility.

15



LEGEND

- ◆ PROPOSED MONITORING WELL LOCATION
- ⊕ EXISTING MONITORING WELL LOCATION
- ⊞ EXISTING EXTRACTION WELL LOCATION



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FIGURE 6

PROPOSED MONITORING WELL LOCATION

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5.0 REFERENCES

- Anderson, M., and W.W. Woessner, 1992. *Applied Groundwater Modeling; Simulation of Flow and Advective Transport*. Academic Press. San Diego, California.
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APPENDIX A
PROCESSES AND MATHEMATICAL STATEMENT

IGWMC GROUNDWATER MODELING SOFTWARE

SOLUTE

**A Program Package of Analytical Models for
Solute Transport in Groundwater**

by

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Hydrolink, Inc., Cincinnati, Ohio
for
Holcomb Research Institute,
Butler University

BAS 15
Version 2.0
July 1989
Released March 1990

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INTRODUCTION

During the last decade, the problem of groundwater pollution has emerged as one of the most critical environmental issues of our time. Pollutants originate from many different sources, including agricultural, industrial, and energy production activities, and the prediction of their movement in groundwater is a major challenge facing groundwater specialists and water resource managers. Solute transport models are designed to meet this challenge by simulating the subsurface migration of various solutes.

Once the governing equations and the initial and boundary conditions are defined, two solution methods are available: analytical and numerical. A number of assumptions are necessary to obtain an analytical solution of the advection-dispersion equation. One generally must assume a constant groundwater velocity, a constant coefficient of dispersion, constant physical parameters, and a simplified geometry of the system. Consequently, because analytical models appear to be of limited use for field situations, most investigators have turned to numerical models, disregarding analytical models. However, analytical solutions are useful in analyzing the sensitivity of a model to variations in input parameters. In many field situations few data are available and numerical solutions are of limited use because of many uncertainties. The advantages of analytical models are ease of application and low cost of operation.

The program package "SOLUTE" contains the analytical solutions of one-dimensional advection-dispersion equations (ONED1 and ONED3), two-dimensional advection-dispersion equations in uniform groundwater flow (PLUME2D and SLUG2D), in radial groundwater flow (RADIAL and LTIRD), and three-dimensional advection-dispersion equations (PLUME3D and SLUG3D). In addition, the package includes the program UNITS that will be appreciated by anyone who works with groundwater units of measure. The programs are menu-driven and easy to use.

This documentation is divided into two parts: the first part is theoretical and presents the general advection-dispersion equation and its parameters; the second part contains the program documentation with the mathematical model, and the assumptions for each program.

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I. PROCESSES AND MATHEMATICAL STATEMENT

NOTATION

$Ai(x)$	Airy function of x
b	aquifer thickness, L
C	solute concentration, M/L^3
S	adsorbed concentration, M/L^3
C'	concentration in a source or sink fluid, M/L^3
CD	dimensionless concentration
D	hydrodynamic dispersion coefficient, L^2/T
D_{ij} or D	dispersion coefficient tensor, L^2/T
D_L, D_T	longitudinal and transverse dispersion coefficients, L^2/T
D_x, D_y, D_z	dispersion coefficient in the x, y , and z directions, L^2/T
D^*	molecular diffusion coefficient, L^2/T
$erf(x)$	error function of x , equal to $\left[\left(2/\sqrt{\pi} \right) \int_0^x e^{-z^2} dz \right]$
$erfc(x)$	complementary error function, equal to $1 - erf(x)$
$exp(x)$	exponential of x , equal to e^x
g	gravitational acceleration, L/T^2
h	hydraulic head, L
K	hydraulic conductivity, L/T
K_{ij}	hydraulic conductivity tensor, L/T
K_d	distribution coefficient relating C and S
n	effective porosity
Q	rate of recharge or discharge, L^3/T
q	specific discharge or Darcy velocity, L/T
R	retardation factor
r	radial distance, L
r_D	dimensionless radius
r_{Dw}	dimensionless well radius
s	parameter of Laplace transformation, $1/T$
S_s	specific storage, $1/L$
t	time, T
t_D	dimensionless time
t_o	period of activity of a source, T
\bar{v}_{gw}	average pore water velocity or seepage velocity, L/T
\bar{v}	vector of average pore water velocity, L/T
\bar{v}_i	average pore water velocity in the direction i , L/T
\bar{v}_s	contaminant velocity, L/T
W^*	volume flow rate per unit volume of a source or sink, $1/T$
x	x coordinate, L
x_i	Cartesian coordinate, L

y	y coordinate, L
z	z coordinate, L
α	decay factor of a source, $1/T$
α_L	longitudinal dispersivity, L
α_T	transverse or lateral dispersivity, L
λ	radioactive decay constant, equal to $\ln 2$ /half-life; $1/T$
ρ_b	bulk density of solid, M/L^3

PROCESSES AND MATHEMATICAL STATEMENT

Groundwater flow through the individual pores of an aquifer cannot be described in an exact mathematical form. Instead, the real, complex system of solids and pores (voids) is replaced by the concept of a porous medium or continuum. The porous medium is a portion of space occupied by heterogeneous or multiphase material, with at least one of the phases a solid phase or a solid matrix. The domain not occupied by the solid matrix is the pore space.

At every point of the continuum, variables, such as groundwater velocity, pressure, and concentration that describe the state of the system, form continuous fields. The information about the complex geometry of the void-solid interface is replaced by solid matrix parameters such as porosity, permeability, and dispersivity. The value of any property (whether of the solid matrix or the fluid in the void space) at any point in the continuum is an average taken over some representative elementary volume (REV) around that point (Bear 1972). The REV concept allows moving from the microscopic level of description to the macroscopic. Although most of the flow and transport models are at the macroscopic level, understanding the phenomena that occur in a porous medium must be at the microscopic level. The models are developed on the basis of a water balance (flow models) or a mass balance of a solute (transport models).

ADVECTION-DISPERSION EQUATION

Mass conservation of a solute is expressed by the partial differential equation (Anderson 1979):

$$\underbrace{\frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C}{\partial x_j} \right)}_{\text{[dispersion]}} - \underbrace{\frac{\partial}{\partial x_i} (C \bar{v}_i)}_{\text{[advection]}} - \underbrace{\frac{C' W^*}{n}}_{\text{[sink/source]}} = \frac{\partial C}{\partial t} \quad (1.1)$$

where C is the concentration of the solute, C' is the concentration of solute in the source or sink fluid, D_{ij} is the dispersion coefficient, a second-order tensor, \bar{v}_i is the seepage velocity or average pore velocity, and W^* is the volume flow rate per unit volume.

Because advective transport and hydrodynamic dispersion both depend on the velocity of groundwater flow, the mathematical model must solve two simultaneous partial differential equations: one is the flow equation from which the hydraulic head, h , is obtained, and the other is the solute transport equation from which the concentration of the solute in groundwater is obtained. The seepage velocity, \bar{v}_i , is calculated from

$$\bar{v}_i = - \frac{K_{ij}}{n} \frac{\partial h}{\partial x_j} \quad (1.2)$$

where n is the effective porosity and K_{ij} is the hydraulic conductivity tensor. The concentration is assumed to be low, so the density or mass per unit volume of the fluid may be considered constant.

Decay

Solutes may undergo radioactive or biological decay as they are transported through the porous medium. The decay is expressed by the equation

$$\frac{\partial C}{\partial t} = -\lambda C \quad (1.3)$$

where λ is the first-order decay constant of the solute and can be calculated if the half-life of the solute $t_{1/2}$ is known

$$\lambda = \frac{\ln(2)}{t_{1/2}} \quad (1.4)$$

Equation (1.1) with the included decay term becomes

$$\frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (C \bar{v}_i) - \frac{C' W^*}{n} - \lambda C = \frac{\partial C}{\partial t} \quad (1.5)$$

Adsorption

The solute under consideration may also undergo chemical reactions and/or adsorption on the surface of the solid phase. If equilibrium-controlled ion exchange reactions are considered, equation (1.5) may be expressed as

$$\frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (C \bar{v}_i) - \frac{C' W^*}{n} - \lambda \left(C + \frac{\rho_b}{n} S \right) = \frac{\partial}{\partial t} \left(C + \frac{\rho_b}{n} S \right) \quad (1.6)$$

where ρ_b is the bulk density of the solid, and S is the concentration of solute adsorbed on the solid surface (mass of solute on the solid phase per unit mass of solid phase).

Isotherms define the equilibrium relationship between the concentrations of adsorbed and dissolved constituents. Equilibrium models assume instantaneous adsorption and desorption of the solute. The most frequently used isotherms are (van Genuchten 1981)

$$\text{Linear} \quad S = k_1 C + k_2 \quad (1.7)$$

$$\text{Langmuir} \quad S = \frac{k_1 C}{1 + k_2 C} \quad (1.8)$$

$$\text{Freundlich} \quad S = k_1 C^{k_2} \quad (1.9)$$

where k_1 and k_2 are empirically derived constants. All adsorption models represent reversible adsorption reactions. Generally, two or more transport equations have to be solved for multi-ion transport problems. The simplest form of the linear isotherm is given as

$$S = K_d C \quad (1.10)$$

where K_d is the distribution coefficient:

$$K_d = \frac{\text{mass of solute on the solid phase per unit mass of solid phase}}{\text{concentration of solute in solution}}$$

Incorporating equation (1.10) into the advection–dispersion equation (1.6) and adding the source/sink fluid term yields the following expression:

$$\frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} \left(C \bar{v}_i \right) - \lambda RC - \frac{C'W^*}{n} = R \frac{\partial C}{\partial t} \quad (1.11)$$

where C' is the concentration of solute in the source/sink fluid, and R is the retardation factor defined by

$$R = 1 + \frac{\rho_b}{n} K_d \quad (1.12)$$

As the result of sorption, solute transport is retarded with respect to that caused by advection and dispersion. For R values that are orders of magnitude larger than unity the solute is essentially immobile, while $R = 1$ indicates that no sorption occurs.

HYDRODYNAMIC DISPERSION

The processes that control the migration of a solute are advection, hydrodynamic dispersion, geochemical and biochemical reactions, and radioactive and biological decay (Bear 1979).

Advection refers to the transport of solute with flowing groundwater. In the case of a conservative solute, no reactions such as adsorption occur between the solute and the solid phase, and the rate of transport is equal to the seepage velocity. If the transport of solute is due only to advection, a sharp interface separates the flow domain that contains the solute and the native groundwater. However, this interface does not remain sharp due to hydrodynamic dispersion, which causes solute spread over a greater volume of the aquifer than would be predicted by an analysis of groundwater velocity.

The coefficient of hydrodynamic dispersion D'_{ij} has two components:

$$D'_{ij} = D_{ij} + D^* \quad (2.1)$$

where D_{ij} is the coefficient of mechanical dispersion, a second-order tensor, and D^* is the coefficient of molecular diffusion. In the domain of normal groundwater velocities, the contribution of molecular diffusion to hydrodynamic dispersion is small compared to mechanical dispersion and may be neglected for any practical purpose (Bear 1979).

The coefficient of mechanical dispersion is proportional to the velocity of groundwater and to the coefficient α_{ijmn} , a fourth-order tensor called dispersivity. Scheidegger (1961) derived the following relation:

$$D_{ij} = \alpha_{ijmn} \frac{\bar{V}_m \bar{V}_n}{|\bar{V}|} \quad (2.2)$$

where \bar{V}_m and \bar{V}_n are components of the flow velocity of groundwater in the m and n directions, and $|\bar{V}|$ is the magnitude of the velocity vector.

For an isotropic porous medium, α_{ijmn} is related to two constants: α_L , longitudinal dispersivity, and α_T , transverse or lateral dispersivity of the porous medium:

$$\alpha_{ijmn} = \alpha_T \delta_{im} \delta_{jn} = \frac{\alpha_L - \alpha_T}{2} (\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}) \quad (2.3)$$

where δ_{ij} is the Kronecker delta. Combining equations (2.2) and (2.3) results in the following expression:

$$D_{ij} = \alpha_T \bar{V} \delta_{ij} + (\alpha_L - \alpha_T) \frac{\bar{V}_i \bar{V}_j}{\bar{V}} \quad (2.4)$$

or in Cartesian coordinates with velocity components \bar{V}_x and \bar{V}_y ,

$$D_{xx} = \alpha_T \bar{V} + (\alpha_L - \alpha_T) \frac{\bar{V}_x^2}{\bar{V}} \quad (2.5a)$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T) \frac{\bar{V}_x \bar{V}_y}{\bar{V}} \quad (2.5b)$$

$$D_{yy} = \alpha_T \bar{V} + (\alpha_L - \alpha_T) \frac{\bar{V}_y^2}{\bar{V}} \quad (2.5c)$$

$$D_{zz} = \alpha_T \bar{V} \quad (2.5d)$$

If one of the axes coincides with the direction of the average uniform velocity $|\bar{V}|$, for example the x-axis, equations (2.5a-d) become

$$D_L = D_{xx} = \alpha_L |\bar{V}| \quad (2.6a)$$

$$D_T = D_{yy} = D_{zz} = \alpha_T |\bar{V}| \quad (2.6b)$$

where D_L and D_T are the coefficients of longitudinal and transverse dispersion, respectively.

When measured in a laboratory sand column, dispersivity is on the order of a few centimeters, but field measurements result in dispersivity on the order of a meter to a hundred meters, depending on the scale of the experiment. The difference between dispersivity values measured in the laboratory and in the field may be attributed to the effects of heterogeneity and anisotropy of the aquifer. Macroscopic dispersion is influenced by spatial variations in hydraulic conductivity fields (Smith and Schwartz 1980). Peaudecerf (1978) collected all published values of dispersivity and showed that dispersivity tends to increase with both the scale of the problem and time. Gelhar et al. (1979) indicate that for a large time span the value of dispersivity approaches some maximum asymptotic value.

Because of the difficulties in measuring dispersivity, both longitudinal and lateral dispersivities are often determined during calibration of the model. The common assumption is that the medium is isotropic with respect to dispersivity, and this implies isotropy with respect to hydraulic conductivity.

INITIAL AND BOUNDARY CONDITIONS

The general initial condition of the advection–dispersion equation is written as

$$C = f(x,y,z), \quad (t = 0) \quad (3.1)$$

where $f(x,y,z)$ can be a constant or some known function.

There are three types of boundary conditions (Javandel et al. 1984):

Dirichlet or First-type Boundary Condition

$$C = C_0(x,y,z,t) \quad (3.2)$$

where $C_0(x,y,z,t)$ is a given function for the particular portion of the boundary. Examples for this type of boundary condition are (1) specified concentration on the boundary of the aquifer, (2) zero concentration on the boundary far from the contaminant source, and (3) specified concentration at injection wells.

Neumann or Second-type Boundary Condition

$$\left(D_{ij} \frac{\partial C}{\partial x_j} \right) n_i = g(x,y,z,t) \quad (3.3)$$

where $g(x,y,z,t)$ is a known function (specified solute flux) and n_i are components of the unit vector normal to the boundary. Typical examples are (1) zero normal concentration gradient on impervious boundaries and (2) known value of solute flux on the boundaries.

Cauchy or Third-type Boundary Condition

$$\left(D_{ij} \frac{\partial C}{\partial x_j} - C \bar{V}_i \right) n_i = q(x,y,z,t) \quad (3.4)$$

where $q(x,y,z,t)$ is a solute flux, a known function. The first term on the left-hand side of the equation represents flux by dispersion, and the second term represents the advection effect. Examples include (1) specified mass flux of contaminant at injection wells, and (2) specified mass flux of contaminant from streams, landfills, and so forth.

II. USER'S MANUAL

SYSTEM REQUIREMENTS

SOLUTE is available in a compiled form for the IBM PC/XT/AT, PS/2 or compatible DOS microcomputer with 640K memory. An EGA/VGA graphics board and a math coprocessor are required. A printer and the HP 7475A plotter are optional.

The programs in the package are written in Microsoft QuickBASIC. The compiled version of the code is distributed by IGWMC.

GETTING STARTED

We assume that the user is familiar with the PC-DOS or MS-DOS commands. The DOS commands are shown in **BOLD CAPITAL LETTERS**.

Before you run the SOLUTE program package, check the directory of the SOLUTE diskette. It should contain the following executable codes:

1. SOLUTE.EXE - executable code for the main-menu
2. ONED.EXE - one-dimensional models
3. PLUME2D.EXE - two-dimensional models
4. RADIAL.EXE - 2-D (radial coordinates) models
5. PLUME3D.EXE - three-dimensional models
6. UNITS.EXE - a utility program.

In addition you should find six input datasets (*.DAT) from the example problems following each program.

If any file is missing or the diskette is damaged, please contact the distributor or the author of the SOLUTE program package.

Before proceeding any further, make a working (backup) copy of the master SOLUTE diskette. Put the original master diskette in a safe place and use the copy from now on. If the copy is ever damaged or destroyed, you can always make a new copy from the original diskette.

For a System with Two Disk Drives

Only the high-density 5-1/4" SOLUTE version or a 3-1/2" SOLUTE disk will work. If you obtained SOLUTE on double density disks, copy contents of both disks to your hard disk.

To start the program, place the SOLUTE diskette in drive A and the working disk (a disk where you will be saving data and output files) in drive B. To invoke the SOLUTE program, type:

A:\ SOLUTE

The introductory screen will be displayed. After pressing any key you should see the MAIN MENU of the SOLUTE program on your screen.

For a System with a Hard Disk

The following optional DOS command constantly display the current default directory at the DOS prompt (if you like this feature you can add this command to the AUTOEXEC.BAT file):

```
C:> PROMPT $P$G
```

Make a directory named SOLUTE (or any other name) on the hard disk (in the given example it is C drive):

```
C:> MD SOLUTE
```

Make the SOLUTE Directory the current directory:

```
C:> CD SOLUTE
```

Place the SOLUTE diskettes in A drive and copy all files from the diskette to the directory:

```
C:\SOLUTE> COPY A:*.*
```

To invoke the SOLUTE program, type:

```
C:\SOLUTE> SOLUTE
```

The introductory screen will be displayed. After pressing any key you should see the MAIN MENU of the SOLUTE program displayed on your screen.

MENU OPTIONS

Each program in the SOLUTE package is menu-driven. The main menu has the following options:

- | | |
|---------------------------|---------------------------|
| 1. ENTER new data | 6. DISPLAY results |
| 2. READ data from a file | 7. PLOT on screen |
| 3. EDIT current data | 8. PRINT output |
| 4. WRITE data to a file | 9. SAVE results to a file |
| 5. COMPUTE concentrations | 10. DOS shell |
| 0. EXIT to select model | |

Enter New Data

This option allows you to enter input data interactively. The data can be in metric or English units. If you enter a wrong value, you can always change it later using the editor (OPTION 3). The program will ask you questions and if you give an unacceptable answer, the program will stare at you and will wait for an acceptable answer.

Read Data from a File

When asked for the name of the data file, give the full name of the file including the disk drive letter and the path. The program will read the file and return to the MAIN MENU.

If you have forgotten the name of the file, press < ENTER > . The program will ask you for the disk drive and the path of the directory where you saved the data file. It will then search that directory for all files with extension ".DAT". All such files will be displayed on the screen and you can load the desired file by entering the corresponding number of the file. If the specified directory does not contain a single file with the extension, the program will return to the MAIN MENU without reading a file.

Edit Current Data

This option allows you to change the input data that you have just entered (OPTION 1) or read (OPTION 2).

Write Data to a File

Before you exit a SOLUTE program, you can save the entered data in an external file. The disk drive and the path must be included in the name of the file, or else the data will be saved in the current directory. A good practice is to give the data files the extension .DAT (for example RUN55.DAT).

Compute Concentrations

Once you have entered all input data, select this option to calculate concentrations at the specified distances. When the computation is done the program will return to the MAIN MENU. To display results in a tabular form select OPTION 6; to display a screen graph select OPTION 7.

Display Results

This option (OPTION 6) allows you to view results in a tabular form on the screen.

Plot on Screen

This option (OPTION 7) allows you to plot the results from the run on the screen. To return to the MAIN MENU press any key.

Print Output

The input data and results can be printed by selecting this option (OPTION 8).

Save Results to a File

Most users have a commercial graphics package for X-Y plots or contouring. This option (OPTION 9) allows you to save the results of the run in an ASCII file in the X, Y- or X, Y, Z-format so that you can read the saved file in any graphics package that would take the format (most programs do).

DOS Shell

This option allows you to exit the program temporarily to the DOS level and enter any DOS command (PRINT, DIR, CHKDSK, etc.). This is a handy option if you want to print a file, check what files are in the directory, or check the amount of space on a diskette, for example. To return to the program, you must enter the command:

C:\SOLUTE > EXIT

This will bring you back to the MAIN MENU.

Exit to Main Menu

To end the program and return to the MAIN MENU, select this option (OPTION 0).

PROGRAM DOCUMENTATION

PROGRAMS IN SOLUTE PACKAGE

No.	Name	Description
1	ONED1	One-dimensional solute transport in a semi-infinite column, constant concentrations as the inlet boundary condition.
2	ONED3	One-dimensional solute transport in a semi-infinite column, specified mass flux as the inlet boundary condition. Retardation and decay options included.
3	PLUME2D	Two-dimensional transport of a plume from continuous multiple point sources in a uniform groundwater flow field. Includes options for retardation and decay.
4	SLUG2D	Two-dimensional transport of a slug from an instantaneous point source in a uniform groundwater flow field.
5	RADIAL	Solute transport in a plane radial flow. This program calculates the concentration distribution along the radial coordinate from a recharge well.
6	LTIRD	Same as RADIAL, but based on improved solution of solute transport equation in radial coordinates.
7	PLUME3D	Three-dimensional solute transport of a plume from continuous multiple point sources in a uniform groundwater flow field. Decay option included.
8	SLUG3D	Three-dimensional transport of a slug from an instantaneous point source in a uniform groundwater flow field. Decay option included.
9	UNITS	This program converts the most frequently used units in hydrogeology from English units to metric units and vice versa.

PLUME2D

PROGRAM IDENTIFICATION

Program Title: Analytical Model for Transport of a Solute Plume from Point Sources in a Uniform Two-Dimensional Groundwater Flow Field

Program Code Name: PLUME2D

Programmer: Milovan S. Beljin

Program Organization: International Ground Water Modeling Center
Holcomb Research Institute, Butler University
Indianapolis, Indiana 46208, USA. Tel: 317/283-9458

Date: January 1989

Version: 2.00

Source Language: Microsoft QuickBASIC 4.0

Memory Requirements: 320K

Availability: PLUME2D is a nonproprietary code distributed by IGWMC.
A copy of the program on a 5-1/4" or 3-1/2" diskette is available.

Abstract: A program to calculate the concentration distribution of a plume from point sources in two-dimensional regional flow. It includes options for retardation and decay.

Comments: PLUME2D is based on the Wilson and Miller (1978) equation.

PLUME2D

MATHEMATICAL MODEL

If a pollutant is injected continuously from a point source into an aquifer, a plume develops downstream from the source and spreads out to the sides. If the aquifer is relatively thin, vertical mixing occurs, and the concentration becomes uniform throughout the thickness of the aquifer; i.e., the plume is two-dimensional. The governing equation and initial and boundary conditions for this problem are

$$D_{xx} \frac{\partial^2 C}{\partial x^2} + D_{yy} \frac{\partial^2 C}{\partial y^2} - \bar{v} \frac{\partial C}{\partial x} - \lambda RC + \frac{Q_c}{n} = R \frac{\partial C}{\partial t} \quad (3.3.1)$$

$$C(x, y, 0) = 0 \quad (3.3.2)$$

$$Q_c(x, y, t) = Q C_0 \delta(x, y) \quad (3.3.3)$$

$$C(\pm \infty, \pm \infty, t) = 0 \quad (3.3.4)$$

where

- Q_c = the mass injection rate of solute per unit volume of aquifer
- Q = the volumetric injection rate of fluid per unit of aquifer thickness
- C_0 = concentration of the injected fluid
- $\delta(x, y)$ = the Dirac delta function

The analytical solution of the problem is given in the form (Hunt 1978, Wilson and Miller 1978)

$$C(x, y, t) = \frac{Q C_0 \exp(x/B)}{4 \pi n \sqrt{D_{xx} D_{yy}}} W(u, r/B) \quad (3.3.5)$$

where

$$B = \frac{2 D_{xx}}{\bar{v}} \quad (3.3.6)$$

$$r = \left[\left(x^2 + \frac{D_{xx}}{D_{yy}} y^2 \right) Y \right]^{1/2} \quad (3.3.7)$$

$$Y = 1 + \frac{2 B \lambda R}{\bar{v}} \quad (3.3.8)$$

$$u = \frac{r^2 R}{4 Y D_{xx} t} \quad (3.3.9)$$

$$W(u, r/B) = \int_u^{\infty} \frac{1}{\Theta} \exp \left[-\Theta - \frac{r^2}{4B^2\Theta} \right] d\Theta \quad (3.3.10)$$

The function $W(u, r/B)$ corresponds to the Hantush well function for the problem of transient flow to a well in an infinite leaky aquifer. Hantush (1956) tabulated values of the function for the given arguments, but for many pollution problems the ratio r/B is large and tabulated values are insufficient. Wilson and Miller (1978) approximate the function as follows:

$$W(u, r/B) \approx \left(\frac{\pi B}{2r} \right)^{1/2} \exp(-r/B) \operatorname{erfc} \left(-\frac{r/B - 2u}{2\sqrt{u}} \right) \quad (3.3.11)$$

The approximation is reasonably accurate (within 10 percent) for $r/B > 1$ and more accurate (within one percent) for $r/B > 10$ (Wilson and Miller 1978).

As a check on the accuracy of this function, the value of r/B (for the given distance downstream from the source) should be calculated before the approximation is applied.

In practice the problem described corresponds to that involving the movement of a continuously injected solute into an aquifer from a fully penetrating recharge well. The additional assumptions of the analytical models are that (a) the aquifer is homogeneous, isotropic, infinite in areal extent, and constant in thickness; (b) recharge rates are negligible relative to the uniform regional flow rate; and (c) the solute is distributed instantaneously over the entire aquifer thickness.

As $t \rightarrow \infty$ and $u \rightarrow 0$, a steady-state condition arises between the rate of solute dispersion and the rate of injection. In that case the following equation can be applied to calculate the concentration distribution:

$$C(x, y, t) = \frac{Q C_0 \exp(x/B)}{2\pi n \sqrt{D_{xx} D_{yy}}} K_0(r/B) \quad (3.3.12)$$

where K_0 is the modified Bessel function of the second kind and order zero.

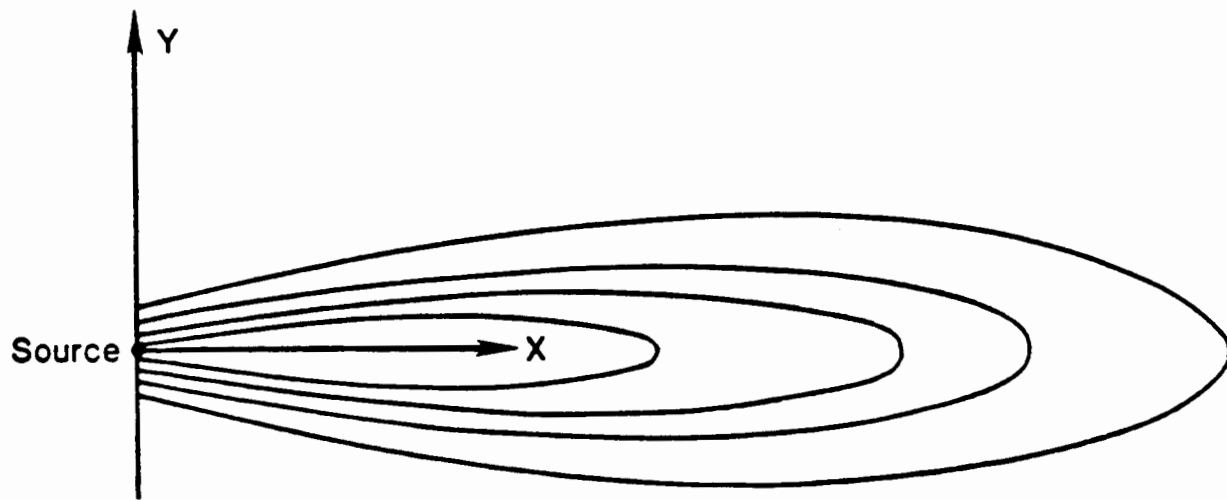
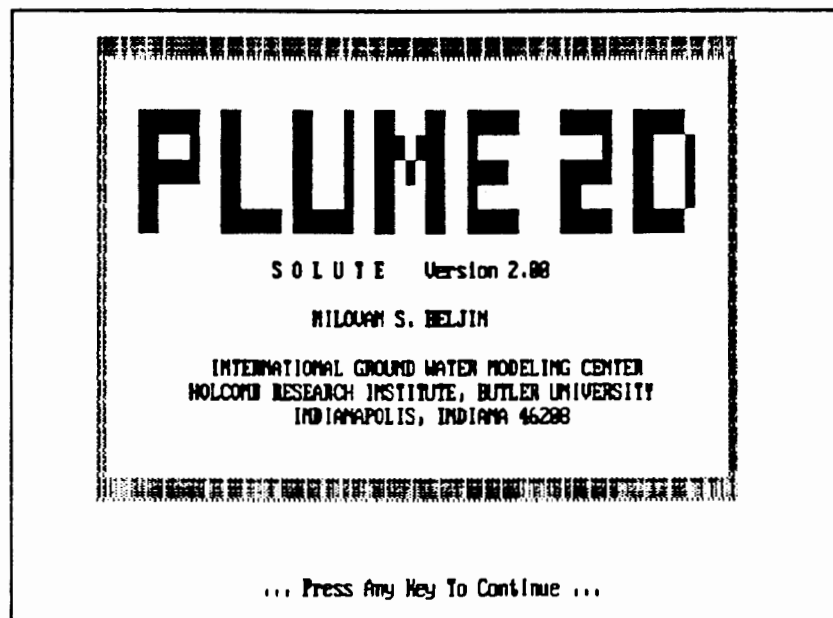


Figure 3. Plume from a point source.

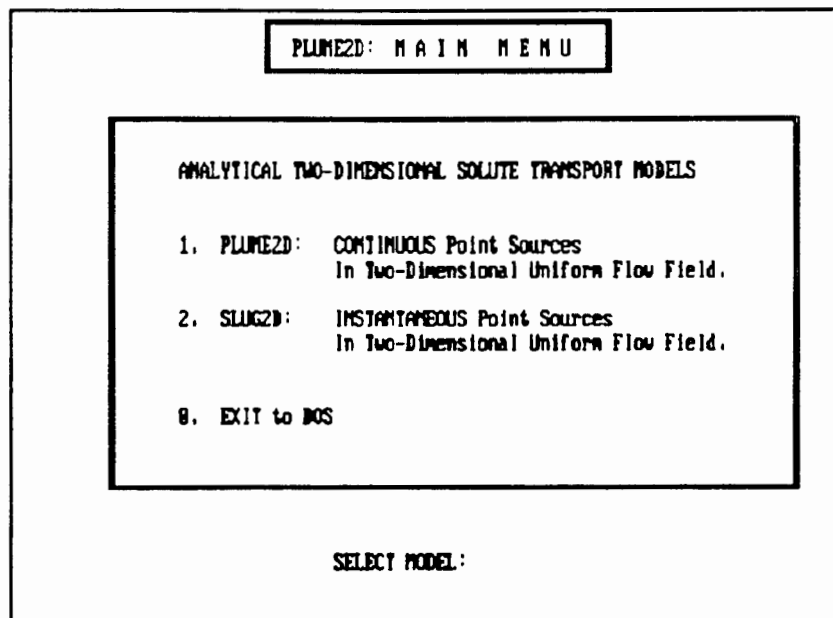
ASSUMPTIONS OF PLUME2D MODEL:

- uniformly porous confined aquifer
- the aquifer is homogeneous, isotropic, infinite in areal extent, and constant in thickness
- a fully penetrating solute injection well
- recharge rates are negligible in relation to uniform regional flow rate
- pollutants are distributed instantaneously to the entire aquifer thickness beneath the point source
- injection is continuous and constant.

EXAMPLE PROBLEM



PLUME2D: Execution Sequence



PLUME2D: EDITING DATA

1. PROJECT TITLE (max 15 char.)..... = J. Hyd. Div.
2. USER NAME..... = IGMC
3. DATE..... = 09-25-1989
4. GROUNDWATER VELOCITY..... = .46 (m/d)
5. AQUIFER THICKNESS..... = 33.5 (m)
6. POROSITY..... = .35
7. LONGITUDINAL DISPERSIVITY..... = 21.3 (m)
8. LATERAL DISPERSIVITY..... = 4.3 (m)
9. RETARDATION FACTOR..... = 1
10. HALF-LIFE..... = 0 (d)
11. NUMBER OF POINT SOURCES..... = 1

To continue: press <ENTER>. To edit: type line number :

PLUME2D: EDITING DATA

SOURCE NO. 1

1. X-COORDINATE OF THE SOURCE..... = 0 (m)
2. Y-COORDINATE OF THE SOURCE..... = 0 (m)
3. SOURCE STRENGTH..... = 23.6 (kg/d)
4. ELAPSED TIME..... = 2888 (d)

To continue: press <ENTER>. To edit: type line number :

PLUME2D: EDITING DATA

GRID DATA:

1. X-COORDINATE OF GRID ORIGIN..... = 0 (m)
2. Y-COORDINATE OF GRID ORIGIN..... = 0 (m)
3. DISTANCE INCREMENT DELX..... = 200 (m)
4. DISTANCE INCREMENT DELY..... = 50 (m)
5. NUMBER OF MODES IN X-DIRECTION... = 15
6. NUMBER OF MODES IN Y-DIRECTION... = 9

To continue: press <ENTER>, To edit: type line number :

PLUME2D: Results

CONCENTRATION C (mg/l)

ROW\COLUMN (m)	1 0.00	2 200.00	3 400.00	4 600.00	5 800.00
1 0.00	-1.0000	42.0907	29.7605	24.2609	20.6537
2 50.00	4.1400	19.9770	20.4407	18.9151	17.1279
3 100.00	0.2140	3.3507	7.1707	9.1060	9.0665
4 150.00	0.0129	0.3557	1.5210	2.9500	4.0560
5 200.00	0.0000	0.0312	0.2303	0.6022	1.2343
6 250.00	0.0001	0.0025	0.0279	0.1211	0.2007
7 300.00	0.0000	0.0002	0.0029	0.0175	0.0536
8 350.00	0.0000	0.0000	0.0003	0.0021	0.0001
9 400.00	0.0000	0.0000	0.0000	0.0002	0.0010

... Press Any Key To Continue ...

PLUME2D: Results

CONCENTRATION C [mg/l]

ROW\COLUMN [m]	6 1000.00	7 1200.00	8 1400.00	9 1600.00	10 1800.00
1 0.00	16.7635	11.1070	5.8316	1.3687	0.2023
2 50.00	14.3762	9.6975	4.4334	1.2040	0.1796
3 100.00	9.1872	6.4652	3.8353	0.8366	0.1257
4 150.00	4.3135	3.3890	1.6106	0.4561	0.0694
5 200.00	1.5536	1.3103	0.6747	0.1956	0.0363
6 250.00	0.4335	0.4049	0.2200	0.0661	0.0104
7 300.00	0.0953	0.0905	0.0570	0.0177	0.0020
8 350.00	0.0167	0.0190	0.0116	0.0037	0.0006
9 400.00	0.0024	0.0029	0.0019	0.0006	0.0001

... Press Any Key To Continue ...

PLUME2D: Results

CONCENTRATION C [mg/l]

ROW\COLUMN [m]	11 2000.00	12 2200.00	13 2400.00	14 2600.00	15 2800.00
1 0.00	0.0150	0.0006	0.0000	0.0000	0.0000
2 50.00	0.0140	0.0006	0.0000	0.0000	0.0000
3 100.00	0.0099	0.0004	0.0000	0.0000	0.0000
4 150.00	0.0055	0.0002	0.0000	0.0000	0.0000
5 200.00	0.0024	0.0001	0.0000	0.0000	0.0000
6 250.00	0.0000	0.0000	0.0000	0.0000	0.0000
7 300.00	0.0002	0.0000	0.0000	0.0000	0.0000
8 350.00	0.0001	0.0000	0.0000	0.0000	0.0000
9 400.00	0.0000	0.0000	0.0000	0.0000	0.0000

... Press Any Key To Continue ...

III. REFERENCES

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PLUME2D

PROGRAM IDENTIFICATION

Program Title: Analytical Model for Transport of a Solute Plume from Point Sources in a Uniform Two-Dimensional Groundwater Flow Field

Program Code Name: PLUME2D

Programmer: Milovan S. Beljin

Program Organization: International Ground Water Modeling Center
Holcomb Research Institute, Butler University
Indianapolis, Indiana 46208, USA. Tel: 317/283-9458

Date: January 1989

Version: 2.00

Source Language: Microsoft QuickBASIC 4.0

Memory Requirements: 320K

Availability: PLUME2D is a nonproprietary code distributed by IGWMC.
A copy of the program on a 5-1/4" or 3-1/2" diskette is available.

Abstract: A program to calculate the concentration distribution of a plume from point sources in two-dimensional regional flow. It includes options for retardation and decay.

Comments: PLUME2D is based on the Wilson and Miller (1978) equation.

PLUME2D

MATHEMATICAL MODEL

If a pollutant is injected continuously from a point source into an aquifer, a plume develops downstream from the source and spreads out to the sides. If the aquifer is relatively thin, vertical mixing occurs, and the concentration becomes uniform throughout the thickness of the aquifer; i.e., the plume is two-dimensional. The governing equation and initial and boundary conditions for this problem are

$$D_{xx} \frac{\partial^2 C}{\partial x^2} + D_{yy} \frac{\partial^2 C}{\partial y^2} - \bar{v} \frac{\partial C}{\partial x} - \lambda RC + \frac{Q_c}{n} = R \frac{\partial C}{\partial t} \quad (3.3.1)$$

$$C(x, y, 0) = 0 \quad (3.3.2)$$

$$Q_c(x, y, t) = Q C_0 \delta(x, y) \quad (3.3.3)$$

$$C(\pm \infty, \pm \infty, t) = 0 \quad (3.3.4)$$

where

- Q_c = the mass injection rate of solute per unit volume of aquifer
- Q = the volumetric injection rate of fluid per unit of aquifer thickness
- C_0 = concentration of the injected fluid
- $\delta(x, y)$ = the Dirac delta function

The analytical solution of the problem is given in the form (Hunt 1978, Wilson and Miller 1978)

$$C(x, y, t) = \frac{Q C_0 \exp(x/B)}{4 \pi n \sqrt{D_{xx} D_{yy}}} W(u, r/B) \quad (3.3.5)$$

where

$$B = \frac{2 D_{xx}}{\bar{v}} \quad (3.3.6)$$

$$r = \left[\left(x^2 + \frac{D_{xx}}{D_{yy}} y^2 \right) Y \right]^{1/2} \quad (3.3.7)$$

$$Y = 1 + \frac{2 B \lambda R}{\bar{v}} \quad (3.3.8)$$

$$u = \frac{r^2 R}{4 Y D_{xx} t} \quad (3.3.9)$$

$$W(u, r/B) = \int_u^\infty \frac{1}{\Theta} \exp \left[-\Theta - \frac{r^2}{4B^2\Theta} \right] d\Theta \quad (3.3.10)$$

The function $W(u, r/B)$ corresponds to the Hantush well function for the problem of transient flow to a well in an infinite leaky aquifer. Hantush (1956) tabulated values of the function for the given arguments, but for many pollution problems the ratio r/B is large and tabulated values are insufficient. Wilson and Miller (1978) approximate the function as follows:

$$W(u, r/B) \approx \left(\frac{\pi B}{2r} \right)^{1/2} \exp(-r/B) \operatorname{erfc} \left(-\frac{r/B - 2u}{2\sqrt{u}} \right) \quad (3.3.11)$$

The approximation is reasonably accurate (within 10 percent) for $r/B > 1$ and more accurate (within one percent) for $r/B > 10$ (Wilson and Miller 1978).

As a check on the accuracy of this function, the value of r/B (for the given distance downstream from the source) should be calculated before the approximation is applied.

In practice the problem described corresponds to that involving the movement of a continuously injected solute into an aquifer from a fully penetrating recharge well. The additional assumptions of the analytical models are that (a) the aquifer is homogeneous, isotropic, infinite in areal extent, and constant in thickness; (b) recharge rates are negligible relative to the uniform regional flow rate; and (c) the solute is distributed instantaneously over the entire aquifer thickness.

As $t \rightarrow \infty$ and $u \rightarrow 0$, a steady-state condition arises between the rate of solute dispersion and the rate of injection. In that case the following equation can be applied to calculate the concentration distribution:

$$C(x, y, t) = \frac{Q C_0 \exp(x/B)}{2\pi n \sqrt{D_{xx} D_{yy}}} K_0(r/B) \quad (3.3.12)$$

where K_0 is the modified Bessel function of the second kind and order zero.

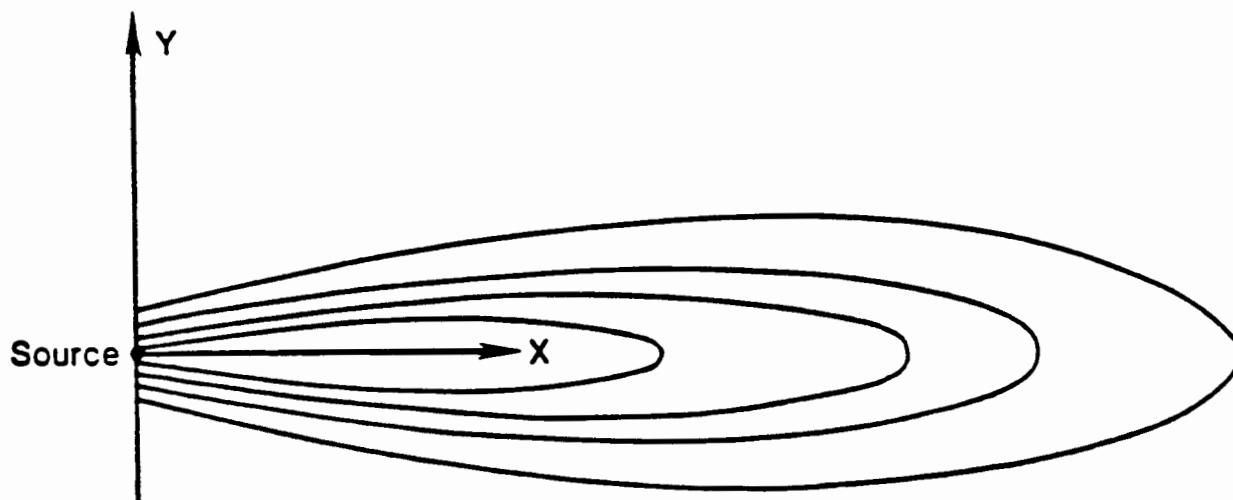
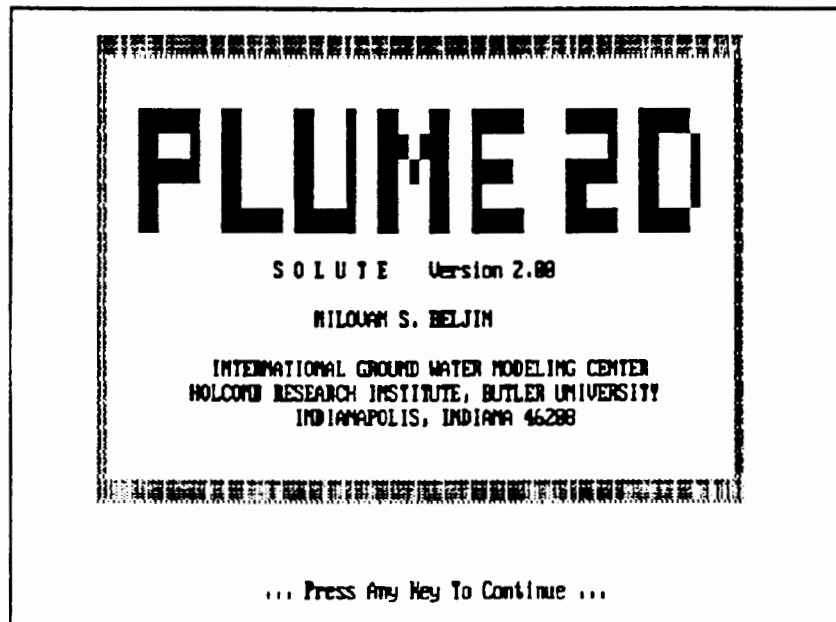


Figure 3. Plume from a point source.

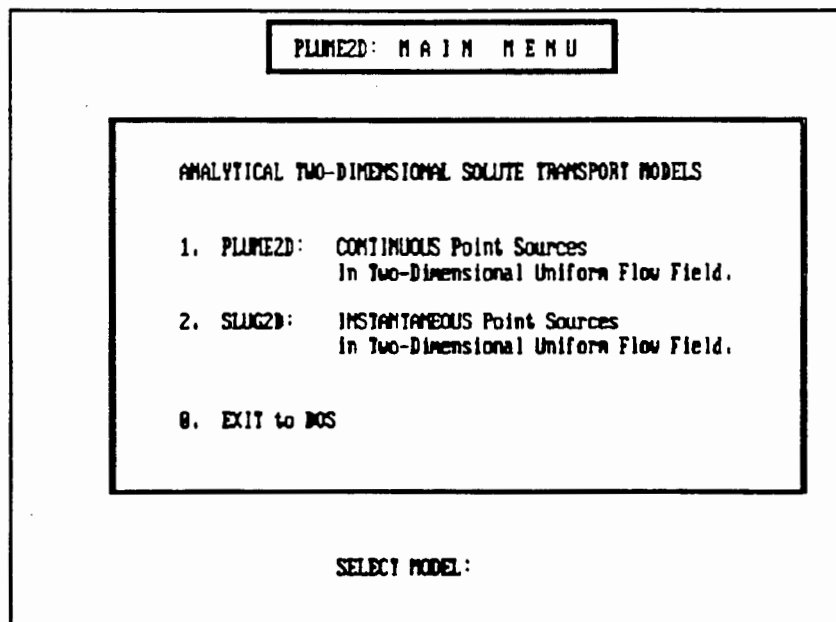
ASSUMPTIONS OF PLUME2D MODEL:

- uniformly porous confined aquifer
- the aquifer is homogeneous, isotropic, infinite in areal extent, and constant in thickness
- a fully penetrating solute injection well
- recharge rates are negligible in relation to uniform regional flow rate
- pollutants are distributed instantaneously to the entire aquifer thickness beneath the point source
- injection is continuous and constant.

EXAMPLE PROBLEM



PLUME2D: Execution Sequence



PLUFE2D: EDITING DATA

1. PROJECT TITLE (max 15 char.)..... = J. Hyd. Div.
2. USER NAME..... = IGWPC
3. DATE..... = 09-25-1989
4. GROUNDWATER VELOCITY..... = .46 (m/d)
5. AQUIFER THICKNESS..... = 33.5 (m)
6. POROSITY..... = .35
7. LONGITUDINAL DISPERSIVITY..... = 21.3 (m)
8. LATERAL DISPERSIVITY..... = 4.3 (m)
9. RETARDATION FACTOR..... = 1
10. HALF-LIFE..... = 0 (d)
11. NUMBER OF POINT SOURCES..... = 1

To continue: press <ENTER>. To edit: type line number :

PLUFE2D: EDITING DATA

SOURCE NO. 1

1. X-COORDINATE OF THE SOURCE..... = 0 (m)
2. Y-COORDINATE OF THE SOURCE..... = 0 (m)
3. SOURCE STRENGTH..... = 23.6 (kg/d)
4. ELAPSED TIME..... = 2000 (d)

To continue: press <ENTER>. To edit: type line number :

PLUME2D: EDITING DATA

GRID DATA:

1. X-COORDINATE OF GRID ORIGIN..... = 0 (m)
2. Y-COORDINATE OF GRID ORIGIN..... = 0 (m)
3. DISTANCE INCREMENT DELX..... = 200 (m)
4. DISTANCE INCREMENT DELY..... = 50 (m)
5. NUMBER OF MODES IN X-DIRECTION... = 15
6. NUMBER OF MODES IN Y-DIRECTION... = 9

To continue: press <ENTER>. To edit: type line number :

PLUME2D: Results

CONCENTRATION C (mg/l)

ROW\COLUMN (m)	1	2	3	4	5
	0.00	200.00	400.00	600.00	800.00
1 0.00	-1.0000	42.0907	29.7605	24.2609	20.6537
2 50.00	4.1400	19.9770	20.4407	18.9151	17.1279
3 100.00	0.2140	3.3507	7.1707	9.1060	9.0665
4 150.00	0.0129	0.3557	1.5210	2.9500	4.0560
5 200.00	0.0000	0.0312	0.2303	0.6022	1.2343
6 250.00	0.0001	0.0025	0.0279	0.1211	0.2007
7 300.00	0.0000	0.0002	0.0029	0.0175	0.0536
8 350.00	0.0000	0.0000	0.0003	0.0021	0.0081
9 400.00	0.0000	0.0000	0.0000	0.0002	0.0010

... Press Any Key To Continue ...

PLUME2D: Results

		CONCENTRATION C (mg/l)				
ROW\COLUMN (n)		6	7	8	9	10
		1000.00	1200.00	1400.00	1600.00	1800.00
1	0.00	16.7635	11.1878	5.8316	1.3687	0.2023
2	50.00	14.3762	9.6975	4.4334	1.2948	0.1796
3	100.00	9.1872	6.4652	3.8353	0.8366	0.1257
4	150.00	4.3135	3.3898	1.6186	0.4561	0.0694
5	200.00	1.5536	1.3183	0.6747	0.1956	0.0383
6	250.00	0.4335	0.4049	0.2208	0.0661	0.0184
7	300.00	0.0953	0.0985	0.0578	0.0177	0.0028
8	350.00	0.0167	0.0198	0.0116	0.0037	0.0006
9	400.00	0.0024	0.0029	0.0019	0.0006	0.0001

... Press Any Key To Continue ...

PLUME2D: Results

		CONCENTRATION C (mg/l)				
ROW\COLUMN (n)		11	12	13	14	15
		2000.00	2200.00	2400.00	2600.00	2800.00
1	0.00	0.0158	0.0006	0.0000	0.0000	0.0000
2	50.00	0.0148	0.0006	0.0000	0.0000	0.0000
3	100.00	0.0099	0.0004	0.0000	0.0000	0.0000
4	150.00	0.0055	0.0002	0.0000	0.0000	0.0000
5	200.00	0.0024	0.0001	0.0000	0.0000	0.0000
6	250.00	0.0008	0.0000	0.0000	0.0000	0.0000
7	300.00	0.0002	0.0000	0.0000	0.0000	0.0000
8	350.00	0.0001	0.0000	0.0000	0.0000	0.0000
9	400.00	0.0000	0.0000	0.0000	0.0000	0.0000

... Press Any Key To Continue ...

APPENDIX B
MODELING OUTPUT

```
*****
*
*   INTERNATIONAL GROUND WATER MODELING CENTER
*   INDIANAPOLIS. INDIANA - DELFT. NETHERLANDS
*
*           S O L U T E   1-2-3
*
*   ANALYTICAL MODELS FOR SOLUTE TRANSPORT
*
*****
```

PROJECT..... = SCC Run1
USER NAME..... = DSA
DATE..... = 08-12-1993
DATA FILE..... = c:\junk\run1.dat

INPUT DATA:

GROUNDWATER (SEEPAGE) VELOCITY.... = 3.74 [ft/d]
AQUIFER THICKNESS..... = 73 [ft]
POROSITY..... = .3
LONGITUDINAL DISPERSIVITY..... = 20 [ft]
LATERAL DISPERSIVITY..... = 2 [ft]
RETARDATION FACTOR..... = 1
HALF-LIFE..... = 0 [d]
NUMBER OF POINT SOURCES..... = 1

SOURCE NO. 1

X-COORDINATE OF THE SOURCE.... = 0 [ft]
Y-COORDINATE OF THE SOURCE.... = 0 [ft]
SOURCE STRENGTH..... = 4.73 [lb/d]
ELAPSED TIME..... = 3650 [d]

GRID DATA:

X-COORDINATE OF GRID ORIGIN..... = 0 [ft]
Y-COORDINATE OF GRID ORIGIN..... = 0 [ft]
DISTANCE INCREMENT DELX..... = 10 [ft]
DISTANCE INCREMENT DELY..... = 10 [ft]
NUMBER OF NODES IN X-DIRECTION.... = 21
NUMBER OF NODES IN Y-DIRECTION.... = 15

CONCENTRATION C [mg/l]

ROW\COLUMN			1	2	3	4	5
[ft]			0.00	10.00	20.00	30.00	40.00
1	0.00	[ft]	-1.0000	58.3504	41.2599	33.6886	29.1752
2	10.00	[ft]	14.8835	17.9544	19.5170	19.8982	19.6325
3	20.00	[ft]	4.7736	5.9733	7.1143	8.1133	8.9290
4	30.00	[ft]	1.7679	2.2342	2.7368	3.2551	3.7686
5	40.00	[ft]	0.6945	0.8816	1.0941	1.3284	1.5797
6	50.00	[ft]	0.2817	0.3586	0.4483	0.5510	0.6658
7	60.00	[ft]	0.1167	0.1487	0.1868	0.2314	0.2826
8	70.00	[ft]	0.0490	0.0625	0.0788	0.0981	0.1208
9	80.00	[ft]	0.0208	0.0265	0.0335	0.0420	0.0519
10	90.00	[ft]	0.0089	0.0114	0.0144	0.0180	0.0224
11	100.00	[ft]	0.0038	0.0049	0.0062	0.0078	0.0097
12	110.00	[ft]	0.0017	0.0021	0.0027	0.0034	0.0042
13	120.00	[ft]	0.0007	0.0009	0.0012	0.0015	0.0018
14	130.00	[ft]	0.0003	0.0004	0.0005	0.0006	0.0008
15	140.00	[ft]	0.0001	0.0002	0.0002	0.0003	0.0004

ROW\COLUMN			6	7	8	9	10
[ft]			50.00	60.00	70.00	80.00	90.00
1	0.00	[ft]	26.0951	23.8214	22.0544	20.6300	19.4501
2	10.00	[ft]	19.0794	18.4253	17.7573	17.1135	16.5090
3	20.00	[ft]	9.5573	10.0175	10.3378	10.5472	10.6709
4	30.00	[ft]	4.2601	4.7169	5.1315	5.5003	5.8233
5	40.00	[ft]	1.8423	2.1105	2.3790	2.6430	2.8986
6	50.00	[ft]	0.7918	0.9274	1.0708	1.2203	1.3738
7	60.00	[ft]	0.3405	0.4050	0.4757	0.5522	0.6339
8	70.00	[ft]	0.1469	0.1767	0.2101	0.2473	0.2881
9	80.00	[ft]	0.0636	0.0771	0.0926	0.1101	0.1298
10	90.00	[ft]	0.0276	0.0337	0.0408	0.0489	0.0582
11	100.00	[ft]	0.0120	0.0148	0.0180	0.0217	0.0260
12	110.00	[ft]	0.0053	0.0065	0.0079	0.0096	0.0116
13	120.00	[ft]	0.0023	0.0028	0.0035	0.0043	0.0052
14	130.00	[ft]	0.0010	0.0013	0.0015	0.0019	0.0023
15	140.00	[ft]	0.0004	0.0006	0.0007	0.0008	0.0010

ROW\COLUMN		11	12	13	14	15
[ft]		100.00	110.00	120.00	130.00	140.00
1	0.00 [ft]	18.4520	17.5933	16.8443	16.1835	15.5948
2	10.00 [ft]	15.9478	15.4296	14.9515	14.5101	14.1021
3	20.00 [ft]	10.7297	10.7399	10.7142	10.6619	10.5903
4	30.00 [ft]	6.1025	6.3410	6.5428	6.7119	6.8523
5	40.00 [ft]	3.1430	3.3740	3.5906	3.7919	3.9779
6	50.00 [ft]	1.5295	1.6855	1.8405	1.9930	2.1419
7	60.00 [ft]	0.7202	0.8102	0.9033	0.9987	1.0957
8	70.00 [ft]	0.3325	0.3803	0.4311	0.4848	0.5411
9	80.00 [ft]	0.1517	0.1757	0.2020	0.2303	0.2608
10	90.00 [ft]	0.0687	0.0804	0.0934	0.1078	0.1235
11	100.00 [ft]	0.0309	0.0365	0.0429	0.0499	0.0578
12	110.00 [ft]	0.0139	0.0165	0.0195	0.0229	0.0268
13	120.00 [ft]	0.0062	0.0075	0.0089	0.0105	0.0123
14	130.00 [ft]	0.0028	0.0034	0.0040	0.0048	0.0056
15	140.00 [ft]	0.0012	0.0015	0.0018	0.0022	0.0026

ROW\COLUMN		16	17	18	19	20
[ft]		150.00	160.00	170.00	180.00	190.00
1	0.00 [ft]	15.0660	14.5876	14.1520	13.7533	13.3865
2	10.00 [ft]	13.7239	13.3727	13.0456	12.7402	12.4544
3	20.00 [ft]	10.5048	10.4094	10.3074	10.2010	10.0919
4	30.00 [ft]	6.9675	7.0610	7.1356	7.1940	7.2385
5	40.00 [ft]	4.1487	4.3050	4.4473	4.5765	4.6935
6	50.00 [ft]	2.2865	2.4259	2.5598	2.6878	2.8097
7	60.00 [ft]	1.1935	1.2915	1.3892	1.4861	1.5816
8	70.00 [ft]	0.5996	0.6600	0.7220	0.7853	0.8495
9	80.00 [ft]	0.2932	0.3275	0.3635	0.4012	0.4403
10	90.00 [ft]	0.1406	0.1590	0.1787	0.1998	0.2220
11	100.00 [ft]	0.0665	0.0760	0.0863	0.0976	0.1097
12	110.00 [ft]	0.0311	0.0359	0.0411	0.0469	0.0533
13	120.00 [ft]	0.0144	0.0168	0.0194	0.0223	0.0256
14	130.00 [ft]	0.0067	0.0078	0.0091	0.0105	0.0121
15	140.00 [ft]	0.0031	0.0036	0.0042	0.0049	0.0057

ROW\COLUMN		21
[ft]		200.00
1	0.00 [ft]	13.0475
2	10.00 [ft]	12.1863
3	20.00 [ft]	9.9814
4	30.00 [ft]	7.2709
5	40.00 [ft]	4.7990
6	50.00 [ft]	2.9254
7	60.00 [ft]	1.6755
8	70.00 [ft]	0.9143
9	80.00 [ft]	0.4807
10	90.00 [ft]	0.2455
11	100.00 [ft]	0.1226
12	110.00 [ft]	0.0602
13	120.00 [ft]	0.0291
14	130.00 [ft]	0.0139
15	140.00 [ft]	0.0066

```
*****
*
*      INTERNATIONAL GROUND WATER MODELING CENTER      *
*      INDIANAPOLIS. INDIANA - DELFT. NETHERLANDS      *
*
*      S O L U T E   1-2-3                             *
*
*      ANALYTICAL MODELS FOR SOLUTE TRANSPORT           *
*
*****
```

PROJECT..... = SCC Run2
USER NAME..... = DSA
DATE..... = 08-12-1993
DATA FILE..... = c:\junk\run2.dat

INPUT DATA:

GROUNDWATER (SEEPAGE) VELOCITY.... = .77 [ft/d]
AQUIFER THICKNESS..... = 73 [ft]
POROSITY..... = .3
LONGITUDINAL DISPERSIVITY..... = 10 [ft]
LATERAL DISPERSIVITY..... = 1 [ft]
RETARDATION FACTOR..... = 1
HALF-LIFE..... = 0 [d]
NUMBER OF POINT SOURCES..... = 1

SOURCE NO. 1

X-COORDINATE OF THE SOURCE..... = 0 [ft]
Y-COORDINATE OF THE SOURCE..... = 0 [ft]
SOURCE STRENGTH..... = .7 [lb/d]
ELAPSED TIME..... = 3650 [d]

GRID DATA:

X-COORDINATE OF GRID ORIGIN..... = 0 [ft]
Y-COORDINATE OF GRID ORIGIN..... = 0 [ft]
DISTANCE INCREMENT DELX..... = 10 [ft]
DISTANCE INCREMENT DELY..... = 10 [ft]
NUMBER OF NODES IN X-DIRECTION.... = 21
NUMBER OF NODES IN Y-DIRECTION.... = 15

ROW\COLUMN			11	12	13	14	15
[ft]			100.00	110.00	120.00	130.00	140.00
1	0.00	[ft]	18.7576	17.8846	17.1232	16.4515	15.8530
2	10.00	[ft]	14.3496	14.0318	13.7195	13.4167	13.1257
3	20.00	[ft]	6.8992	7.1581	7.3656	7.5300	7.6583
4	30.00	[ft]	2.4088	2.6698	2.9169	3.1486	3.3640
5	40.00	[ft]	0.6911	0.8120	0.9379	1.0668	1.1974
6	50.00	[ft]	0.1763	0.2172	0.2629	0.3131	0.3673
7	60.00	[ft]	0.0418	0.0536	0.0674	0.0833	0.1016
8	70.00	[ft]	0.0095	0.0125	0.0162	0.0207	0.0261
9	80.00	[ft]	0.0021	0.0028	0.0038	0.0049	0.0064
10	90.00	[ft]	0.0005	0.0006	0.0008	0.0011	0.0015
11	100.00	[ft]	0.0001	0.0001	0.0002	0.0003	0.0003
12	110.00	[ft]	0.0000	0.0000	0.0000	0.0001	0.0001
13	120.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
14	130.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
15	140.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000

ROW\COLUMN			16	17	18	19	20
[ft]			150.00	160.00	170.00	180.00	190.00
1	0.00	[ft]	15.3155	14.8292	14.3864	13.9811	13.6082
2	10.00	[ft]	12.8474	12.5819	12.3292	12.0887	11.8599
3	20.00	[ft]	7.7566	7.8301	7.8829	7.9186	7.9400
4	30.00	[ft]	3.5631	3.7462	3.9139	4.0671	4.2065
5	40.00	[ft]	1.3283	1.4582	1.5862	1.7115	1.8335
6	50.00	[ft]	0.4252	0.4863	0.5501	0.6161	0.6838
7	60.00	[ft]	0.1220	0.1448	0.1697	0.1968	0.2258
8	70.00	[ft]	0.0324	0.0397	0.0480	0.0574	0.0679
9	80.00	[ft]	0.0081	0.0102	0.0127	0.0156	0.0190
10	90.00	[ft]	0.0020	0.0025	0.0032	0.0040	0.0050
11	100.00	[ft]	0.0005	0.0006	0.0008	0.0010	0.0013
12	110.00	[ft]	0.0001	0.0001	0.0002	0.0002	0.0003
13	120.00	[ft]	0.0000	0.0000	0.0000	0.0001	0.0001
14	130.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
15	140.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000

ROW\COLUMN			21
			[ft]
			200.00
1	0.00	[ft]	13.2636
2	10.00	[ft]	11.6420
3	20.00	[ft]	7.9495
4	30.00	[ft]	4.3332
5	40.00	[ft]	1.9518
6	50.00	[ft]	0.7528
7	60.00	[ft]	0.2568
8	70.00	[ft]	0.0796
9	80.00	[ft]	0.0229
10	90.00	[ft]	0.0062
11	100.00	[ft]	0.0016
12	110.00	[ft]	0.0004
13	120.00	[ft]	0.0001
14	130.00	[ft]	0.0000
15	140.00	[ft]	0.0000

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*****
*
*   INTERNATIONAL GROUND WATER MODELING CENTER   *
*   INDIANAPOLIS, INDIANA - DELFT, NETHERLANDS  *
*
*               S O L U T E   1-2-3              *
*
*   ANALYTICAL MODELS FOR SOLUTE TRANSPORT        *
*
*****
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PROJECT..... = SCC Run3
USER NAME..... = DSA
DATE..... = 08-12-1993
DATA FILE..... = c:\junk\run3.dat

INPUT DATA:

GROUNDWATER (SEEPAGE) VELOCITY.... = 4.3 [ft/d]
AQUIFER THICKNESS..... = 73 [ft]
POROSITY..... = .3
LONGITUDINAL DISPERSIVITY..... = 30 [ft]
LATERAL DISPERSIVITY..... = 3 [ft]
RETARDATION FACTOR..... = 1
HALF-LIFE..... = 0 [d]
NUMBER OF POINT SOURCES..... = 1

SOURCE NO. 1

X-COORDINATE OF THE SOURCE..... = 0 [ft]
Y-COORDINATE OF THE SOURCE..... = 0 [ft]
SOURCE STRENGTH..... = 6.72 [lb/d]
ELAPSED TIME..... = 3650 [d]

GRID DATA:

X-COORDINATE OF GRID ORIGIN..... = 0 [ft]
Y-COORDINATE OF GRID ORIGIN..... = 0 [ft]
DISTANCE INCREMENT DELX..... = 10 [ft]
DISTANCE INCREMENT DELY..... = 10 [ft]
NUMBER OF NODES IN X-DIRECTION.... = 21
NUMBER OF NODES IN Y-DIRECTION.... = 15

CONCENTRATION C [mg/l]

ROW\COLUMN			1	2	3	4	5
[ft]			0.00	10.00	20.00	30.00	40.00
1	0.00	[ft]	-1.0000	58.8721	41.6288	33.9898	29.4360
2	10.00	[ft]	19.5441	21.9724	22.7673	22.4833	21.7078
3	20.00	[ft]	8.1585	9.4541	10.5604	11.4243	12.0429
4	30.00	[ft]	3.9325	4.5925	5.2435	5.8607	6.4252
5	40.00	[ft]	2.0105	2.3559	2.7165	3.0840	3.4498
6	50.00	[ft]	1.0616	1.2463	1.4450	1.6552	1.8737
7	60.00	[ft]	0.5721	0.6724	0.7824	0.9013	1.0282
8	70.00	[ft]	0.3127	0.3678	0.4290	0.4962	0.5691
9	80.00	[ft]	0.1727	0.2032	0.2375	0.2754	0.3172
10	90.00	[ft]	0.0961	0.1132	0.1324	0.1539	0.1778
11	100.00	[ft]	0.0538	0.0634	0.0743	0.0865	0.1001
12	110.00	[ft]	0.0303	0.0357	0.0418	0.0488	0.0566
13	120.00	[ft]	0.0171	0.0202	0.0237	0.0276	0.0321
14	130.00	[ft]	0.0097	0.0114	0.0134	0.0157	0.0183
15	140.00	[ft]	0.0055	0.0065	0.0076	0.0089	0.0104

ROW\COLUMN			6	7	8	9	10
[ft]			50.00	60.00	70.00	80.00	90.00
1	0.00	[ft]	26.3284	24.0344	22.2515	20.8144	19.6240
2	10.00	[ft]	20.7771	19.8423	18.9624	18.1553	17.4223
3	20.00	[ft]	12.4459	12.6761	12.7757	12.7806	12.7189
4	30.00	[ft]	6.9252	7.3556	7.7171	8.0139	8.2524
5	40.00	[ft]	3.8065	4.1475	4.4682	4.7653	5.0370
6	50.00	[ft]	2.0973	2.3228	2.5472	2.7677	2.9820
7	60.00	[ft]	1.1620	1.3013	1.4448	1.5910	1.7386
8	70.00	[ft]	0.6475	0.7310	0.8189	0.9108	1.0059
9	80.00	[ft]	0.3627	0.4119	0.4646	0.5207	0.5798
10	90.00	[ft]	0.2041	0.2328	0.2640	0.2977	0.3337
11	100.00	[ft]	0.1153	0.1320	0.1503	0.1703	0.1919
12	110.00	[ft]	0.0653	0.0750	0.0858	0.0975	0.1104
13	120.00	[ft]	0.0371	0.0428	0.0490	0.0559	0.0635
14	130.00	[ft]	0.0212	0.0244	0.0281	0.0321	0.0366
15	140.00	[ft]	0.0121	0.0140	0.0161	0.0185	0.0211

ROW\COLUMN			11	12	13	14	15
[ft]			100.00	110.00	120.00	130.00	140.00
1	0.00	[ft]	18.6170	17.7506	16.9949	16.3282	15.7342
2	10.00	[ft]	16.7584	16.1564	15.6090	15.1097	14.6525
3	20.00	[ft]	12.6113	12.4732	12.3155	12.1457	11.9695
4	30.00	[ft]	8.4396	8.5828	8.6887	8.7634	8.8120
5	40.00	[ft]	5.2827	5.5029	5.6984	5.8706	6.0213
6	50.00	[ft]	3.1883	3.3852	3.5717	3.7471	3.9112
7	60.00	[ft]	1.8863	2.0329	2.1773	2.3186	2.4561
8	70.00	[ft]	1.1037	1.2034	1.3045	1.4061	1.5079
9	80.00	[ft]	0.6418	0.7063	0.7731	0.8416	0.9117
10	90.00	[ft]	0.3719	0.4124	0.4549	0.4994	0.5455
11	100.00	[ft]	0.2151	0.2400	0.2665	0.2945	0.3241
12	110.00	[ft]	0.1243	0.1394	0.1557	0.1730	0.1915
13	120.00	[ft]	0.0718	0.0809	0.0907	0.1013	0.1128
14	130.00	[ft]	0.0415	0.0469	0.0528	0.0593	0.0662
15	140.00	[ft]	0.0240	0.0272	0.0307	0.0346	0.0388

ROW\COLUMN			16	17	18	19	20
[ft]			150.00	160.00	170.00	180.00	190.00
1	0.00	[ft]	15.2007	14.7180	14.2786	13.8763	13.5062
2	10.00	[ft]	14.2324	13.8448	13.4860	13.1528	12.8425
3	20.00	[ft]	11.7905	11.6116	11.4344	11.2603	11.0900
4	30.00	[ft]	8.8391	8.8485	8.8433	8.8263	8.7996
5	40.00	[ft]	6.1523	6.2652	6.3620	6.4442	6.5134
6	50.00	[ft]	4.0638	4.2052	4.3357	4.4556	4.5655
7	60.00	[ft]	2.5892	2.7174	2.8404	2.9579	3.0699
8	70.00	[ft]	1.6092	1.7095	1.8084	1.9055	2.0006
9	80.00	[ft]	0.9830	1.0551	1.1278	1.2007	1.2735
10	90.00	[ft]	0.5933	0.6424	0.6928	0.7442	0.7964
11	100.00	[ft]	0.3550	0.3873	0.4208	0.4556	0.4914
12	110.00	[ft]	0.2111	0.2318	0.2535	0.2763	0.3000
13	120.00	[ft]	0.1250	0.1380	0.1518	0.1664	0.1818
14	130.00	[ft]	0.0737	0.0818	0.0904	0.0996	0.1094
15	140.00	[ft]	0.0434	0.0483	0.0537	0.0594	0.0656

ROW\COLUMN			21
			[ft]
			200.00
1	0.00	[ft]	13.1642
2	10.00	[ft]	12.5525
3	20.00	[ft]	10.9242
4	30.00	[ft]	8.7651
5	40.00	[ft]	6.5710
6	50.00	[ft]	4.6659
7	60.00	[ft]	3.1762
8	70.00	[ft]	2.0933
9	80.00	[ft]	1.3460
10	90.00	[ft]	0.8492
11	100.00	[ft]	0.5281
12	110.00	[ft]	0.3247
13	120.00	[ft]	0.1979
14	130.00	[ft]	0.1198
15	140.00	[ft]	0.0721

CONCENTRATION C [mg/l]

ROW\COLUMN			1	2	3	4	5
[ft]			0.00	10.00	20.00	30.00	40.00
1	0.00	[ft]	-1.0000	59.3166	41.9432	34.2465	29.6583
2	10.00	[ft]	6.8627	10.2277	12.8365	14.4015	15.1630
3	20.00	[ft]	0.9984	1.5729	2.2710	3.0342	3.7996
4	30.00	[ft]	0.1677	0.2686	0.4063	0.5823	0.7939
5	40.00	[ft]	0.0299	0.0482	0.0746	0.1108	0.1583
6	50.00	[ft]	0.0055	0.0089	0.0140	0.0212	0.0312
7	60.00	[ft]	0.0010	0.0017	0.0027	0.0041	0.0061
8	70.00	[ft]	0.0002	0.0003	0.0005	0.0008	0.0012
9	80.00	[ft]	0.0000	0.0001	0.0001	0.0002	0.0002
10	90.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
11	100.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
12	110.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
13	120.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
14	130.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
15	140.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000

ROW\COLUMN			6	7	8	9	10
[ft]			50.00	60.00	70.00	80.00	90.00
1	0.00	[ft]	26.5272	24.2159	22.4196	20.9716	19.7722
2	10.00	[ft]	15.4254	15.4030	15.2249	14.9649	14.6652
3	20.00	[ft]	4.5184	5.1619	5.7187	6.1890	6.5794
4	30.00	[ft]	1.0354	1.2987	1.5752	1.8567	2.1364
5	40.00	[ft]	0.2181	0.2904	0.3749	0.4708	0.5767
6	50.00	[ft]	0.0445	0.0616	0.0831	0.1092	0.1402
7	60.00	[ft]	0.0089	0.0127	0.0177	0.0241	0.0321
8	70.00	[ft]	0.0018	0.0026	0.0037	0.0052	0.0071
9	80.00	[ft]	0.0004	0.0005	0.0008	0.0011	0.0015
10	90.00	[ft]	0.0001	0.0001	0.0002	0.0002	0.0003
11	100.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0001
12	110.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
13	120.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
14	130.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000
15	140.00	[ft]	0.0000	0.0000	0.0000	0.0000	0.0000